VII.13 Evaluation of the Potential Environmental Impacts from Large-Scale Use and Production of Hydrogen in Energy and Transportation Applications

Donald J. Wuebbles (Primary Contact), Seth Olsen, Dong Wang, Wenjing Jia
University of Illinois
Department of Atmospheric Sciences
105 S. Gregory St.
Urbana, IL 61801
Phone: (217) 244-1568; Fax: (217) 244-4393
E-mail: wuebbles@illinois.edu

Manvendra K. Dubey, Thom Rahn
Los Alamos National Laboratory
Mail Stop D462
Los Alamos, NM 87545
Phone: (505) 665-3128; Fax: (505) 665-3285
E-mail: dubey@lanl.gov

Angus Rockett
University of Illinois
Department of Materials Science and Engineering
1304 W. Green St.
Urbana, IL 61801
Phone: (217) 333-0417; Fax: (217) 333-2736
E-mail: arockett@uiuc.edu

David Layzell
University of Calgary
Calgary, Alberta, T2N 1N4
Phone: (403) 220-6100; Fax: (403) 220-2400
E-mail: dlayzell@ucalgary.ca

Jae Edmonds
Pacific Northwest National Laboratory
8400 Baltimore Avenue, Suite 201
College Park, MD 20740-2496
Phone: (301) 314-6749; Fax: (301) 314-6760
E-mail: jae@pnl.gov

DOE Technology Development Manager: Fred C. Joseck
Phone: (202) 586-7932; Fax: (202) 586-9811
E-mail: Fred.Joseck@ee.doe.gov

DOE Project Officer: Katie Randolph
Phone: (303) 275-4901; Fax: (303) 275-4753
E-mail: Katie.Randolph@go.doe.gov

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Objectives

The purpose of this project is to systematically identify and examine possible long-term ecological and environmental effects from the production of hydrogen from various energy sources based on the DOE hydrogen production strategy and the use of that hydrogen in transportation and power applications. From these analyses, a comprehensive impact assessment will be developed to provide reliable estimates of hydrogen leakage rates to the environment and criteria pollutants emitted from the distributed and central-scale hydrogen systems that might be deployed in the future. The project will involve modeling, data analysis and field experiments. Specific objectives include analyses to address the following:

- Impact of hydrogen releases on the oxidative capacity of the atmosphere.
- Long-term stability of the ozone layer due to changes in hydrogen emissions.
- Impact of hydrogen emissions and resulting concentrations on climate.
- Impact on microbial ecosystems involved in hydrogen uptake.
- Role of biological impacts in causing indirect effects on the atmosphere and climate.
- Criteria pollutants emitted from distributed and centralized hydrogen production pathways.
- Criteria pollutants emitted given different scenarios of vehicle market penetration.
- Impact of criteria pollutants on human health, air quality, ecosystems and structures under different penetration scenarios.

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) Future Market Behavior
(B) Stove-piped/Siloed Analytical Capability
(C) Inconsistent Data, Assumptions and Guidelines
(D) Suite of Models and Tools

Contribution to Achievement of DOE Systems Analysis Milestones

This project will contribute to achievement of the following DOE milestones from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- **Milestone 11:** Complete environmental analysis of the technology environmental impacts for the hydrogen scenarios and technology readiness. (2Q 2015)

Accomplishments

- Completed development of emissions scenarios based on Intergovernmental Panel on Climate Change (IPCC) growth scenarios and different H_2 fuel cell technology adoption scenarios. These scenarios span a wide range of possible future paths and encompass the high and low IPCC growth scenarios. Combustion related emissions are evaluated for H_2 fuel cell and H_2 internal combustion engine (ICE) technology adoption. H_2 emissions are based on the conversion of all land-based transportation to H_2 fuel and assume a ~2.5% H_2 leakage rate.
- Preliminary Integrated Assessment Model calculations show substantial decreases in 2050 CO_2 radiative forcing and resulting climate effects from the reduction in CO_2 emissions in a fuel cell powered transportation sector when the H_2 is produced without carbon emissions.
- Stratospheric impact simulations are underway with preliminary results showing a 0.9% decrease in global stratospheric ozone for the highest H_2 emitting scenario. This is potentially a significant concern that needs further study. Though these simulations did not directly include the H_2 offset CO_2 reduction, previous published peer-reviewed studies indicate that this reduction will cause an additional slight decrease in stratospheric ozone.
- Tropospheric and regional impact model runs have been completed to evaluate effects on hydroxyl, tropospheric ozone, and other pollutants on surface air quality for these scenarios. For all future growth scenarios air quality metrics generally improve significantly with the H_2 fuel cell technology option (surface O_3 decreases by as much as 15 ppb for the high emissions scenario), however for the H_2 ICE technology option there is much less improvement in air quality (surface O_3 decreases by only 5 ppm).
- Analyses of measurements in Mexico City demonstrate cases of high H_2 concentrations in a current highly polluted urban atmosphere.
- New laboratory H_2 soil uptake studies show a significant non-linear enhancement of soil H_2 uptake with increasing atmospheric H_2 concentrations. This uptake enhancement could provide a large negative feedback on the growth of atmospheric H_2 concentrations expected from an hydrogen-based transportation sector. For the first time, such nonlinear effects are now being considered in new atmospheric impacts studies.
- H_2 embrittlement of metallic structures will not be significant from the expected levels of atmospheric H_2 under a hydrogen-based transportation sector.
- The risk due to oxygen release plumes from H_2 production has been evaluated. These plumes are not likely to be a problem.

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Introduction

There is limited quantitative understanding of the projected market penetration, the changes in emissions avoided or gained upon transitioning to hydrogen-based systems, and on the resulting impacts on the environment. This project is aimed at an end-to-end analysis of the potential ecological and environmental impacts of transitioning to a hydrogen-based society. Our project team is composed of scientists, engineers, and economists that have the right blend of expertise and tools to appropriately attack the issues we will face in this assessment. The purpose of this project is to systematically identify and examine possible near and long-term ecological and environmental effects from the production of hydrogen from various energy sources based on the DOE hydrogen production strategy and the use of that hydrogen in transportation and power applications. This project, wherever possible, uses state-of-the-art numerical modeling tools of the environment and energy system emissions in combination with relevant new and prior measurements and other analyses to assess the understanding of the potential ecological and environmental impacts from hydrogen market penetration. Careful attention is being given to both H_2 technology options and market penetration scenarios developed by DOE, as well as other atmospheric trace gas projections such as the IPCC Special Report on Emissions Scenarios scenarios being used in climate analyses and the decline in halocarbons due to the Montreal Protocol following World Meteorological Organization. In the process, DOE will also be provided with a capability for further assessing current understanding and remaining uncertainties for addressing the potential environmental impacts from hydrogen technologies.

Approach

Using state-of-the-art modeling tools of the energy-technology-economy system along with other analyses, we are evaluating changes in emissions due to hydrogen technologies and uses. We evaluate the effects of hydrogen on climate and on all aspects of atmospheric chemistry and composition using state-of-the-art three-dimensional global and regional models of atmospheric chemistry and physics. Through field and laboratory studies, we will gain new insights into the relationships affecting soil uptake and the impacts on ecosystems. Analyses will be done, under various assumptions of hydrogen concentrations, of the effect of the potential of hydrogen to degrade materials and structures. From these separate but heavily coordinated assessment studies, a comprehensive impact assessment will be developed to provide reliable estimates of hydrogen leakage rates to the environment and criteria pollutants emitted from the distributed and central-scale hydrogen systems that might be deployed in the future.

Results

Scenarios of future emissions of greenhouse and other important atmospheric gases and particles have been developed encompassing different hydrogen technology adoption paths and future growth projections in transitioning to a hydrogen-based transportation sector. Future growth projections are based on the IPCC A1Fi and B1 scenarios which represent the continued heavy use of fossil fuels and a lower fossil fuel intensity path respectively. Two technology adoption paths were evaluated, the first utilizing hydrogen fuel cells in which volatile organic carbon (VOC), oxides of nitrogen (NO_x), and particulate emissions (PM) are reduced and the second representing a transitional scenario where hydrogen is burned in ICEs in which only VOC and PM emissions are reduced. In these scenarios we assumed all land-based transportation was converted to H_2 and an H_2 leakage rate of ~2.5%. The A1Fi and B1 scenarios are the high and low range of the IPCC scenarios and in conjunction with the two technology adoption alternatives span a wide range of possible future paths.

Three-dimensional tropospheric and regional model simulations of the 2050 atmosphere constrained by the emission scenarios described above have been completed. Analyses of the results reveal that the atmospheric H_2 burden increases under all scenarios, by ~40% for A1Fi and by ~ 25% for B1. Substantial tropospheric O_3 decreases of 7% (A1Fi) and 5% (B1) are realized only for the fuel cell adoption scenarios, while O_3 decreases only slightly (1%) for the H_2 ICE technology scenarios. The oxidizing capacity of the troposphere, as indicated by the tropospheric OH burden, decreases for the fuel cell technology option by 4% for both the A1Fi and B1 scenarios but increases with ICE technology by 6% in the A1Fi and 3% in the B1 scenarios respectively (Table 1). Atmospheric VOC and particulate concentrations decrease in all scenarios.

TABLE 1. Model simulated 2050 annual mean global tropospheric burdens of various gases. Data are for the A1Fi and B1 based emissions scenarios for the Base case (B), fuel cell technology adoption (HS2), and internal combustion technology adoption (HS3). Units are indicated in the column heads for the base scenarios and percent differences for the HS2 and HS3 scenarios.

Scenario	H_2 [ppb]	O_3 [ppb]	CO [ppb]	NOx [ppt]	SO_2 [ppt]	OH [$1e^5/cm^3$]
A1Fi-B	830	44	132	99	44	9
A1Fi-HS2	+39%	-7%	-14%	-16%	-0.5%	-4%
A1Fi-HS3	+40%	-1%	-17%	11%	-1.4%	+6%
B1-B	577	38	90	60	39	10
B1-HS2	+25%	-5%	-4%	-11%	-0.3%	-4%
B1-HS3	+28%	-1%	-7%	+4%	-3.4%	+3%

For the A1Fi fuel cell technology scenario background annual mean surface O_3 decreases by ~10% and up to 50% over some regions (Figure 1). Over the continental U.S., July monthly average O_3 decreases by more than 20% along the coasts and by ~10% in the interior (Figure 2). $PM_{2.5}$ also decreases by ~4% over much of the U.S. with decreases of ~20% over parts of California and the Ohio River Valley (Figure 3). Decreases for the B1 scenario are similar in distribution but smaller in magnitude.

Preliminary results from the stratospheric impact studies show a 0.9% decrease in global stratospheric ozone for the highest H_2 emitting A1Fi scenario. Though these simulations did not directly include the H_2 offset CO_2 reduction, previous studies indicate that

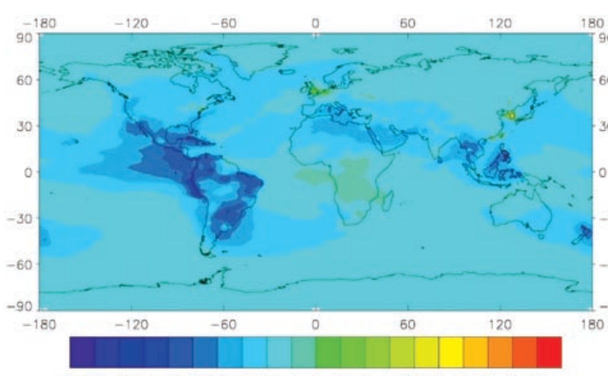

FIGURE 1. Model simulated 2050 annual average percent change in surface ozone for the A1Fi scenario with fuel cell technology adoption (A1Fi-HS2) simulated with the CAM-Chem 3-dimensional global chemistry-transport model.

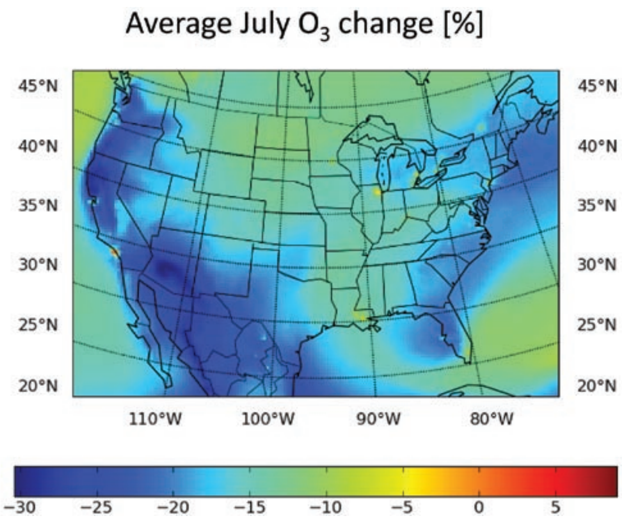

FIGURE 2. July average percent change in surface ozone over the continental U.S. for the A1Fi-HS2 scenario, simulated with the community multiscale air quality model (CMAQ).

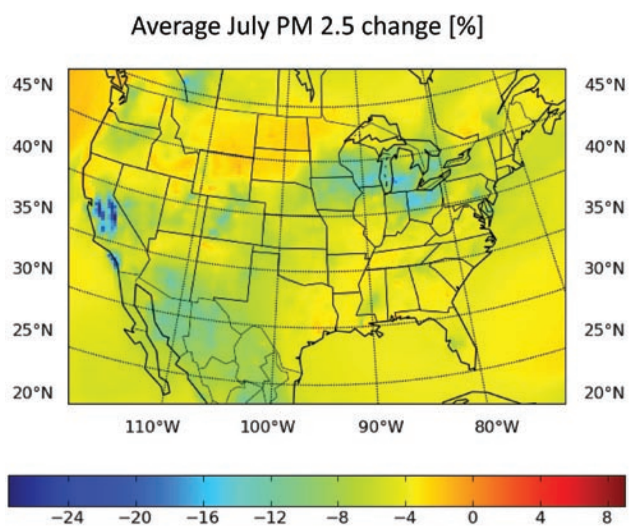

FIGURE 3. July average percent change in $PM_{2.5}$ over the continental U.S. for the A1Fi-HS2 scenario, simulated with CMAQ.

this reduction will cause an additional slight decrease in stratospheric ozone.

Long-term exposure trials indicate that soil H_2 uptake increases with increasing ambient H_2 concentrations. This response could play an important role in determining future H_2 concentrations in a hydrogen economy as demonstrated by our initial studies. The functional dependence of the uptake enhancement has been refined and implemented in our 3-dimensional global tropospheric model. Based on H_2 atmospheric concentrations from our previous A1Fi simulations the uptake may be enhanced by a factor of 4. Full impact studies are underway.

Work on the integrated assessment model is underway. The CO_2 module is complete and analysis of the impact of the displaced CO_2 emissions from conversion to a hydrogen transportation sector indicate that 2050 CO_2 concentrations would be 47 ppm lower for the A1Fi scenario and 21 ppm lower for the B1 scenario. These differences correspond to reduced CO_2 radiative forcings of 0.5 W/m^2 and 0.2 W/m^2 for the A1Fi and B1 scenarios, respectively.

Conclusions and Future Directions

- The tropospheric and regional air quality impacts of an H_2-fueled transportation sector are mostly positive, though for O_3 the impact depends critically on the technology adopted.
- Preliminary results suggest that H_2 causes a decrease in stratospheric O_3. This is a potential concern. These studies and analysis are ongoing.
- The H_2 soil sink depends on the atmospheric H_2 concentration and will likely impact future H_2 concentrations. Further laboratory studies of enhanced H_2 soil uptake dependence on different parameters, e.g., soil type, temperature, and moisture are necessary.
- Global 3-dimensional modeling studies are underway to evaluate the impact of the H_2 adaptive soil sink on future atmospheric H_2 concentrations. The potential importance needs study.
- Reduced atmospheric CO_2 concentrations in an H_2 economy will decrease CO_2 radiative forcing. Development of the integrated assessment model is being completed and the climate impact of various H_2 emissions and adoption scenarios will be evaluated.
- Measurements of H_2 leaks in realistic conditions are badly needed.
- Field studies of total ecosystem response and soil sink as a function of climate parameters are needed.

FY 2009 Publications/Presentations

1. Yanping Cen, Winnie Chan, Neal A. Scott, and David B. Layzell (2009), Soil H_2 uptake in a future hydrogen economy, EOS Trans. AGU, 90(22), Jt. Assem. Suppl., Abstract B73A-08, American Geophysical Union Joint meeting, Toronto, Ontario, Canada, 2009.

2. Olsen, S., D. Wuebbles, D. Wang, W. Jia, and A. Rockett, (2008), Climate and Air Quality Impact of a Hydrogen Economy, Eos Trans. AGU, 89(53), Fall Meet. Suppl., Abstract A21B-0146, Fall American Geophysical Union Meeting, San Francisco, CA, 2008.

3. Dubey M.K., Rahn, T., Olsen, S., and Mazzoleni, C.; The Hydrogen Cycle in Mexico City: Tracing traffic patterns, fingerprinting sources & holiday effects, in preparation for *Atmos. Chem. & Phys.*, 2009.

4. Dubey, M.K., Horowitz, L. et al. Impacts of Global Hydrogen Economy on Air Quality, Oxidative Capacity, and Stratospheric Ozone: MOZART simulations, in preparation for *Int. Journal of Hydrogen Economy*, 2009.

5. Olsen, S., presentation at 2009 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting.