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

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Objectives

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. 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 some 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)
- **Milestone A5:** Output to Systems Integration: Issue report of the environmental analysis of the Hydrogen Program. (4Q, 2015)

Accomplishments

We have completed the following in the first 8 months of the project:

- Completed development of "worst-case" scenario towards determining maximum possible effects on ozone, hydroxyl (oxidative capacity of atmosphere), aerosols, and climate. With development of this scenario, other, more realistic scenarios become straight forward to develop. The "worst-case" scenario assumes that all transportation and power systems using fossil fuels in the Intergovernmental Panel on Climate Change (IPCC) A1FI scenario for 2050 have been converted to hydrogen and that there is an unrealistic 7% leakage rate.
- Initial global tropospheric composition model runs have been done to evaluate effects on hydroxyl, tropospheric ozone and on surface air quality for the "worst-case" scenario. Runs suggest the biggest concern may be effects on the amount of hydroxyl in the troposphere; hydroxyl is referred to as the "cleanser" of the atmosphere. Tropospheriuc ozone decreased in the studies because of the displaced nitrogen oxides (NOx) and hydrocarbon emissions, thus resulting in greatly improved air quality.
- Analyses from measurements in Mexico City demonstrate cases of high hydrogen concentrations in a current highly polluted urban atmosphere.
- Air quality modeling sensitivity studies show the expected effects from reduced transportation emissions of NOx and hydrocarbons, e.g., reduced ozone in NOx-limited regions.
- Soil uptake laboratory studies show a significant increase in soil uptake rates as the amount of atmospheric hydrogen increases, by about a factor of 2. When using this rate in the atmospheric model, the future atmospheric hydrogen decreases significantly, with resulting reduced environmental impacts.
- There are no indications in the literature of a potential ocean sink for hydrogen.
- Evaluation of structures and embrittlement issues suggests that there will be no issue of significance from the expected levels of atmospheric hydrogen under a hydrogen-based society.

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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 hydrogen technology options and market penetration scenarios developed by DOE-Energy Efficiency and Renewable Energy, as well as other atmospheric trace gas projections such as the IPCC Special Report on Emissions Scenarios (SRES) (IPCC, 2000) being used in climate analyses and the decline in halocarbons due to the Montreal Protocol (following WMO, 2007). 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 a state-of-the-art model 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

As a first scenario of future emissions of greenhouse and other important atmospheric gases and particles based on transitioning to a hydrogen-based society, we decided to begin by looking at the largest possible edge of the envelope. We started with the IPCC's SRES called A1FI, which assumes a heavy continued use of fossil fuels through the century (even this scenario assumes that there is a significant transition to alternative energy sources). Working with Jae Edmonds and Hugh Pitcher from Pacific Northwest National Laboratory, we took the energy and transportation use sectors from that scenario and made the assumption that all fossil fuel use in the energy and transportation sectors for the 2050 time period and the 2100 time period transitioned to hydrogen-based technology. In the scenario we assumed that maximum leakage of the hydrogen produced would be 7%. This scenario development provided an excellent experience for the students working on the project to learn about atmospheric emissions and scenario development. This experience will be very valuable as we turn now to more realistic scenarios.

Long-term exposure trials indicate that the assumed first order relationship between pH_2 and soil hydrogen uptake is off by a factor of about 2.0 (range 1.6 to 2.4). In other words, a doubling in pH_2 would result in approximately a 4-fold increase in soil hydrogen uptake. However, there is a lot more complexity in this than was originally thought. We are writing up the results for publication. Bottom line, the modeling studies should include a soil hydrogen adaptation factor of about 2.0X the predicted change in pH_2 (see Figure 1). As mentioned above, we have now tested this in 3-D global modeling studies.

Three-dimensional tropospheric model simulations of 2050 atmosphere constrained by emission scenarios described above have been done. Analyses of results reveal that complete transition of energy and transportation systems to hydrogen-based increases tropospheric hydrogen burden to 7.6 times (1,784 Tg) that under IPCC A1FI scenario projected (234 Tg). If reductions of volatile organic compounds (VOCs) and NOx emissions during fossil fuel burning process are also taken into consideration, this burden is even slightly higher (1,810 Tg). The significant increase in tropospheric hydrogen has great impact on tropospheric OH: tropospheric OH burden decreases by 17% and 23%, without or with VOCs and NOx emissions reduction, respectively. It is also shown that conversion to hydrogen-based society with VOCs and NOx mitigation reduces tropospheric ozone burden by 17%, in which case summer mean surface ozone concentration over continental U.S. would decrease by as much as 35 ppb; while there is no significant change in tropospheric ozone if VOCs and NOx emissions are not reduced (implying that the hydrogen change by itself has little effect on tropospheric ozone). See Table 1 and Figures 2 and 3.

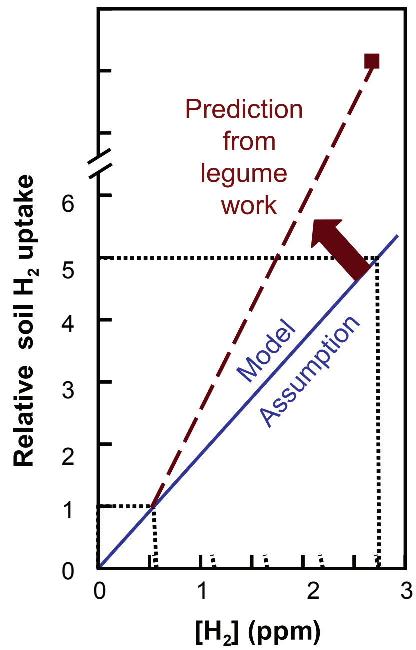

FIGURE 1. Soils respond increases in atmospheric hydrogen by increasing their uptake capacity by more than 5 fold (Range: 8 to 12 fold). Previous global atmospheric models have underestimated by a factor of about 2X, the magnitude of soil feedback in response to elevated pH_2. Adaption factor = 1.6-2.4; best value 2.0.

Model simulations have been carried out under the assumption that soils would adapt to significantly higher ambient hydrogen so that they would uptake twice as much hydrogen. The results suggest that the tropospheric hydrogen burden increases by around 4.2 times (978 Tg and 986 Tg for VOCs and NOx emissions uncontrolled and controlled case, respectively), a lesser extent compared with the scenarios without this assumption. Accordingly, tropospheric OH burden decreases by 9% and 15%, without or with VOCs and NOx emissions reduction, respectively. The effect of VOCs and NOx mitigation on tropospheric ozone is also apparent - tropospheric ozone burden decreases by 19%. Thus, the additional soil uptake of hydrogen has a very significant effect on the perturbation to OH and ozone.

Discussions with the materials experts on the team indicate that the atmospheric levels of hydrogen are unlikely to be large enough to have a significant impact on materials and structures.

TABLE 1. Model simulated 2050 annual mean global tropospheric burdens of various gases, in moles. These are for the "worst-case" scenario relative to the baseline IPCC A1FI scenario. Analyses are presented with and without the increased soil deposition uptake factor.

"Worst-Case" Scenario -- Global Emissions for 2050 (Tg/yr)

- Baseline: A1FI (fossil fuel intensive) IPCC scenario
- Assume that by 2050 all power and transportation globally switched to H_2; assume 7% H_2 leakage
- NOx, VOCs, other emissions greatly reduced

	H_2	NOx	SO_2	CO
A1FI Scenario	54.6	188.2	166.9	1922.4
Hydrogen Society	862.2	36.0	14.3	1029.6

NMVOCs	TOLUENE	CH_3COCH_3	C_2H_6	C_2H_4	C_3H_8	CH_3CHO	MEK	C_2H_5OH	CH_2O	C_3H_6
A1FI Scenario	61.1	30.4	22.2	21.4	20.1	12.7	11.0	8.7	7.1	6.8
Hydrogen Society	8.8	28.4	9.1	19.0	3.4	10.6	8.5	3.6	6.3	5.8

Model Simulated 2050 Annual Mean Global Tropospheric Burdens of Various Gases

Simulations	H_2 (10^{12} mol)	OH (10^6 mol)	NOx (10^9 mol)	O_3 (10^{12} mol)
A1FI (baseline)	116	9.2	14.6	6.3
Hydrogen society without NOx and NMHC reduced	885	7.6	14.6	6.5
Hydrogen society with NOx and NMHC reduced	898	7.1	6.0	5.2
Hydrogen society without NOx and NMHC reduced under soil uptake adaptation assumption*	485	8.4	14.6	6.4
Hydrogen society with NOx and NMHC reduced under soil uptake adaptation assumption*	489	7.8	5.9	5.1

Note: Units are moles
NMHC - non-methane hydrocarbons (used interchangeably with VOCs)
MEK - methyl ethyl ketone
* It is assumed that under high concentration H2 soil deposition uptake would be 2 times as much as the current value.

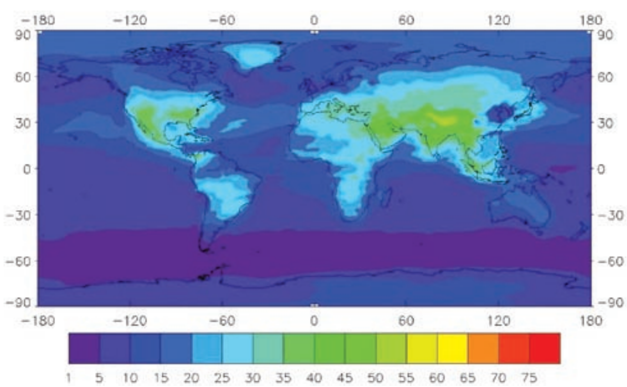

FIGURE 2. 2050 global annual mean surface O_3 concentration under IPCC A1FI scenario (in ppb) derived with the MOZART (Model for OZone And Related Trace species chemical-transport) model.

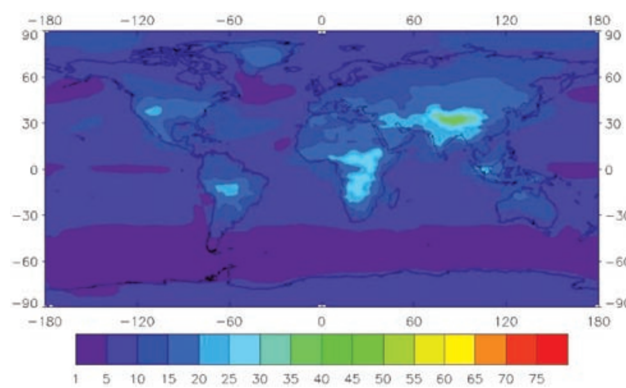

FIGURE 3. 2050 hydrogen society global annual mean surface O_3 concentration (with NOx and non-methane hydrocarbons (NMHC) reduced and soil uptake adaptation assumption) (in ppb) derived with the MOZART model.

Conclusions and Future Directions

Future studies include:

- Complete "worst-case" climate and stratospheric modeling studies.
- Develop "more realistic" scenarios and evaluate parameter space.
- Global chemistry and climate modeling for new scenarios.
- Modeling studies to evaluate soil uptake impact.

- High-resolution urban-scale modeling for the range of scenarios.
- Determine baseline urban hydrogen emissions from oil transport (extend to US metro: Albuquerque).
- Measure leaks in realistic conditions. LANL observations at different locations.
- Ecosystem response and soil sink as a function of climate parameters in Valles Caldera. Incorporate new findings into the modeling studies.
- Development of simplified assessment model.
- Complete report on materials and structures.

FY 2008 Publications/Presentations

1. 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.,* 2008.

2. 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*, 2008.

3. Dubey M.K., Rahn, T., Olsen, S., Mazzoleni, C., and Zhang Y.; The Hydrogen cycle in a megacity: Diurnal Variation, Holiday Effect and Source Fingerprinting, A31C-07, American Geophysical, 22-25 May, Acapulco, Mexico (Eos Trans. AGU, 88(23) A31C-07), 2007.

4. Dubey M.K., Hydrogen Cycle in a Megacity: Diurnal Variation, Holiday Effect and Source Fingerprinting, invited presentation at *Biogeochemistry, Max Planck Institute, Mainz Germany,* 2007.

5. Wuebbles, D., presentation at 2008 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting.