# II.1.5 Hydrogen Effects on Climate, Stratospheric Ozone, and Air Pollution

#### Investigators

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# Introduction

The purpose of this project is to study the potential effects on global and regional climate, stratospheric ozone, and air pollution of replacing fossil-fuel based vehicles and electric power plants with those powered by hydrogen fuel cells, where the hydrogen is produced either from steam reforming of methane, coal gasification, or wind energy. The effects are being estimated with a three-dimensional numerical model of the atmosphere and ocean that is driven by emissions and that treats gases, aerosols, meteorology, clouds, radiation, and surface processes. An important part of the study is the development of emission scenarios for the model simulations.

### Background

Over the last year, two important external papers have been published related to the effects of hydrogen on the atmosphere. In June, 2003, Tromp et al.<sup>1</sup> examined the potential impact of increasing atmospheric hydrogen on stratospheric ozone. They suggested that the addition of hydrogen would increase the abundance of water vapor and cool the stratosphere, a process that would delay recovery of the ozone layer. The primary disadvantages of this paper were that they did not look at the effect of simultaneously reducing fossil-fuel emission, nor did they calculate the climate response of hydrogen itself. In October, 2003, Schultz et al.<sup>2</sup> published a paper examining the effects of a hydrogen economy on tropospheric air chemistry and direct radiative forcing of gases. In their scenarios, they assumed that a reduction in anthropogenic emission would accompany an increase in hydrogen use. They calculated that NOx, CO, and OH would decrease in the global troposphere, and methane would increase upon switching to hydrogen. The increase in methane was estimated to increase global warming (although this was estimated, not calculated). The primary disadvantages of the study were that (1) it did not treat the effects of hydrogen on climate response (e.g., the model did not treat feedback to meteorology but rather simply examined the effects on chemistry and radiative forcing); (2) it did not examine the effects of switching to hydrogen on local or regional pollution (it examined only the large-scale effects); (3) it did not examine the effects of hydrogen on stratospheric ozone; (4) it did not treat aerosols or the effects of hydrogen on them; and (5) the emission scenarios were not resolved to the county or state level.

A few studies have also examined the economic benefits and drawbacks of different methods of producing hydrogen. A recently released DOE study<sup>3</sup> investigated the infrastructure requirements to supply hydrogen to fuel cell vehicles from renewable

resources. The study analyzed the economic and physical feasibility of producing enough hydrogen (10 quads) to supply a 2003-sized vehicle fleet in the year 2004 from renewable electricity sources, in particular, biomass, wind, solar photovoltaic, and geothermal. The study concluded that, among these sources, the most economically attractive and physically available renewable energy resource is wind power, potentially contributing 70.2% of the total energy required across the U.S., and at 40% lower cost than solar photovoltaic. The study also concluded that, in such a future scenario, Class 4 wind resources would be more highly utilized than Class 5 or Class 6 resources because of their proximity to population centers and consequent lower transmission costs. The greater feasibility of Wind Class 4 - generated hydrogen to a future fuel cell vehicle fleet underscores the importance of investigating this scenario for the GCEP study. Bauen et al.<sup>4</sup> have also examined the importance of wind in creating renewable hydrogen for vehicles.

# Results

Between January and May, 2004, several important goals of the project were addressed. An initial goal was to develop emission scenarios for the model simulations. This goal was met with respect to a scenario related to the conversion of the U.S. fleet of onroad vehicles to hydrogen fuel-cell vehicles where the hydrogen is obtained from steam-reforming of methane.

For this scenario, one model simulation will be run with the current fleet of U.S. onroad vehicles and a second simulation will be run with the fleet assuming emission associated with hydrogen fuel cells. Emission data for both the baseline and sensitivity simulation have now been prepared. For the baseline simulation, data for the U.S. were obtained from the U.S. National Emission Inventory, which considers 370,000 stack and fugitive sources, 250,000 area sources, and 1700 categories of onroad and nonroad vehicular sources (including motorcycles, passenger vehicles, trucks, recreational vehicles, construction vehicles, farm vehicles, industrial vehicles, etc.)

An emission inventory for the hydrogen scenario has also been prepared, by Dr. Whitney Colella. Figure 1 illustrates the primary mass, energy, and pollutant flows, as part of a Process Chain Analysis (PCA), in a realistic scenario devised for hydrogen fuel cell vehicles.<sup>5,6,7</sup> In the scenario, hydrogen is derived from natural gas, which is extracted from gas fields, stored, chemically processed, and then transmitted through pipelines to distributed fuel processing units (following, up to this point, the same fuel cycle currently in place for gas turbine power plants and residential heating). The fuel processing units, situated in similar locations as gasoline refueling stations, convert natural gas to hydrogen via a combination of steam reforming and fuel oxidation. Purified hydrogen is then compressed for use onboard fuel cell vehicles.



**Figure 1.** Process Chain Analysis of mass, energy, and pollutant flows in a scenario where hydrogen is obtained from natural gas.

The model simulations to be run require two primary sets of data: (1) the actual emission of gases and particle components associated with hydrogen fuel production and use, and (2) the corresponding reduction in emission associated with reducing fossil fuel use. The quantity of hydrogen-related emission is ultimately a function of the projected hydrogen consumption in on-road vehicles. Figure 2, derived here, shows the estimated

### II.1 Project Results: Hydrogen

annual hydrogen fuel consumption by county in the United States resulting from the replacement of all on-road vehicles with hydrogen fuel-cell vehicles. The data for the figure were obtained by taking the number of miles driven in each U.S. county in 1999 from the U.S. National Emission Inventory, then converting the vehicle-miles travelled into energy requirements for propelling these vehicles (using the average fleet mileage of all on-road vehicles in the NEI's 1999 database of 17.11 miles per gallon and an average gasoline vehicle efficiency of 16% based on Lower Heating Value (LHV) of the fuel), and converting the energy required for propelling the vehicles into hydrogen requirements (using an average hydrogen LHV vehicle efficiency of 53%).<sup>8</sup>

From the hydrogen consumption information, estimates of leaked hydrogen, leaked natural gas, pollutants associated with the steam-reforming process, and pollutants associated with energy required to generate, transport, and compress hydrogen were derived. With respect to hydrogen leakage, we are considering three scenarios: 1%, 5%, and 10% leakage of all hydrogen consumed. Hydrogen leakage can occur during several of the processes in Figure 1. Instead of trying to quantify the actual leakage, which is not possible at this time, we will run scenarios that will provide results based on different assumed leakage rates so that the results can be interpolated once an actual leakage rate is known. With respect to natural gas leakage, we are using a standard estimated rate of 1.0% of additional natural gas consumption, which applies to incremental growth in the U.S. market for currently-available gas transport and processing technologies.<sup>9</sup> With respect to gases emitted during steam-reforming of methane (carbon dioxide and water), we are calculating emission rates based on the stoichiometric ratio of products to reactants in the chemical reactions involved. Steam-reforming also requires energy to generate the steam. We are assuming such energy will come from oxidation of methane fuel. Energy is also needed for other processes. For example, in Figure 1, approximately 10% of the chemical energy (LHV) in the natural gas fuel is needed to produce hydrogen during the (1) exploration (0.7%), (2) production (5.6%), (3) storage and processing (1.0%), and (4) transmission (2.7%) of the gas.<sup>10</sup> We are assuming that this energy is provided by electricity from the current mix of stationary power plants in the U.S. (approximately 51.7% coal, 19.8% nuclear, 15.9% natural gas, 7.2% hydroelectric, 2.8% oil, 2.0% nonhydro renewable, and 0.6% other fossil fuels in 2000).<sup>11</sup> In later stages, energy is also required for hydrogen compression. These net energy inputs are also being derived from the current mix of stationary power plants in the U.S.



**Figure 2:** Map of estimated hydrogen consumption in the U.S. by county if all onroad vehicles were switched to hydrogen fuel-cell vehicles. Light blue=0-5; Medium blue=5-10; Dark blue=10-20; Purple=20-40; Green=40-80; Yellow=80-160; Orange=160-320; Magenta=320-640; Red>640 Gg/yr ( $1Gg=10^9g$ ). See text for discussion.

For the hydrogen scenario, the hydrogen fuel cycle must replace the gasoline fuel cycle, which is based on internal combustion engine vehicles. A gasoline fuel cycle is composed of similar process steps, including exploration, production, processing and refining, and fuel transport via trucks and tankers. Although the gasoline fuel cycle is more energy intensive in the production, refining and transmission stages than is the hydrogen fuel cycle, a first-cut analysis may assume similar levels of energy consumption requirements in the exploration through transmission stages.

Following its transmission stage, the hydrogen fuel cycle requires energy for fuel processing and hydrogen compression, and produces emissions in the form of natural gas leakage, hydrogen leakage, and products of steam-reforming of methane. The gasoline cycle, on the other hand, has fewer energy requirements but produces evaporative emissions of volatile organic compounds and combustion emissions of several pollutants (NO<sub>x</sub>, CO, HCs, CO, PM). In the scenario where gasoline emissions are replaced with hydrogen emissions, evaporative and combustion-related emissions in the U.S. National Emission Inventory will be eliminated.

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Two other tasks of the project in which progress was made during the first stage of this project were (a) developing scenarios for the case where hydrogen is obtained from wind energy and (b) improving the numerical model.

With respect to developing scenarios for wind, two important goals are (i) to locate where wind energy is prevalent and (ii) to locate where wind energy is viable. With these goals in mind Dr. Cristina Archer has been developing a detailed wind map of the United States. Data for the initial map were obtained only from surface and sounding information. Since January, she has obtained additional surface and sounding data to improve the mapping. In addition, she is now examining methods of coupling such data with satellite wind data and model results to fill in gaps where surface and sounding data are not available. Once the mapping is more complete, scenarios will be devised to determine where wind resources will most likely be developed to produce energy for hydrogen.

With respect to model improvements, Gerard Ketefian is improving a 3-D numerical ocean module that will be used in later stages of this project. The module is necessary for determining the long-term effect of changes in greenhouse gases and particles on climate. Since atmospheric perturbations to heating and cooling are diminished by energy diffusion to the deep ocean on a time scale of decades, accounting for the transport of energy to and within the deep ocean is an important goal. The model used for this project, GATOR-GCMOM, currently has a two-dimensional ocean module and treats energy diffusion to the deep ocean with fixed layers below the surface ocean, but energy is not transported in 3-D below the surface layer. As such, the implementation of a 3-D ocean module represents an improvement over what currently exists. It is estimated that the module will be ready for use in 4-8 months.

Model improvements have also been undertaken by M. Jacobson. Specifically, a numerical technique of solving nonequilibrium gas-aerosol transfer of acids and bases simultaneously and among multiple aerosol size bins has been improved. This technique is useful because it allows the solution of such transfer at long time steps with unconditional stability and without numerical oscillation. Growth of acids, such as sulfuric acid, nitric acid, hydrochloric acid, and carbonic acid, and growth of bases, such as ammonia, onto aerosol particles are important because it is a major mechanism of removing such acids from the gas phase, and the aerosols that form as a result have important effects on climate and air quality. The numerical scheme has been tested and will be used in the main model for the hydrogen scenarios.

#### Progress

Emission inventories have been prepared for a realistic hydrogen scenario (replacement of onroad vehicle fuels in the U.S. with hydrogen obtained from steamreforming of methane). Emissions for other scenarios (including hydrogen production from wind) are also in progress. The numerical model to be used for the scenarios has been improved with respect to the treatment of nonequilibrium growth of acids and bases onto aerosol particles. A 3-D ocean module is also being improved.

# **Future Plans**

The next stage of the project is to start running the first computer modeling scenario: a baseline simulation with the current fleet of U.S. onroad vehicles and a second simulation assuming the fleet is converted to vehicles using hydrogen fuel cells, where the hydrogen is obtained from steam-reforming of methane. Concurrently, the hydrogen scenarios will be expanded. Specifically, a scenario in which nonroad vehicles in the U.S. are converted to hydrogen fuel-cell vehicles, and a scenario in which fossil fuel power plants in the U.S. are converged to fuel-cell plants, will be developed. The wind scenario will also be expanded. Ocean model improvements will also continue.

# Publications

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