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

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# Overview

## Timeline

- Start: September 28, 2007
- End: September 27, 2009
- ~20% complete

## Budget

- Total project funding
  - UIUC - $450K
  - LANL - $150K
- Funding received in FY07
  - UIUC - 0
  - LANL - 0
- Funding for FY08
  - UIUC - $180K (expected)
  - LANL - $150K (just arrived)

## Barriers

- Barriers addressed
  - Environmental Quality
  - System Analysis / Environmental Analysis

## Partners

- UIUC - Project lead
- LANL
- PNNL
- Queen's University
- Stanford

# Project Purpose

**The purpose of this project is to systematically identify and examine possible ecological and environmental effects from the production and use of hydrogen from various energy sources based on the DOE hydrogen production strategy and the use of that hydrogen in transportation and power applications.**

# Project Objectives

- **This project uses state-of-the-art numerical models 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.**
- **In the process, DOE will be provided with a capability for further assessing current understanding and remaining uncertainties for addressing the potential environmental impacts from hydrogen technologies.**

# Specific Objectives

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

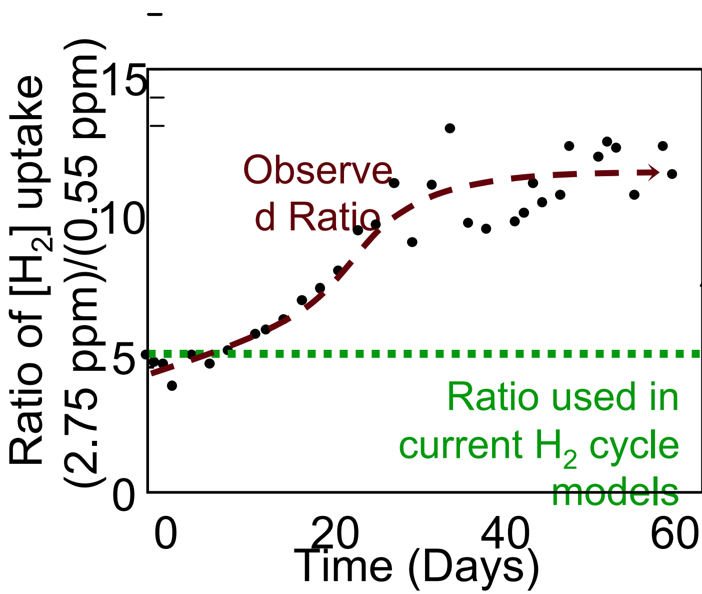
# Project Milestones – FY2008

- **Establish criteria for initial scenario development**
- **Identify and develop U.S. and global scenarios using energy system model.**
- **Assess displaced emissions effects for selected scenarios**
- **With developed scenarios, design the atmospheric model calculations to assess global chemistry and regional air quality effects with and without interactive climate effects.**
- **Initial studies on all objectives.**
- **Summary report of the methodologies used in the assessment**
- **Report on description of model inputs**
- **Interim report on model outputs**
- **Report on the hydrogen and criteria pollutants impact assessment model**

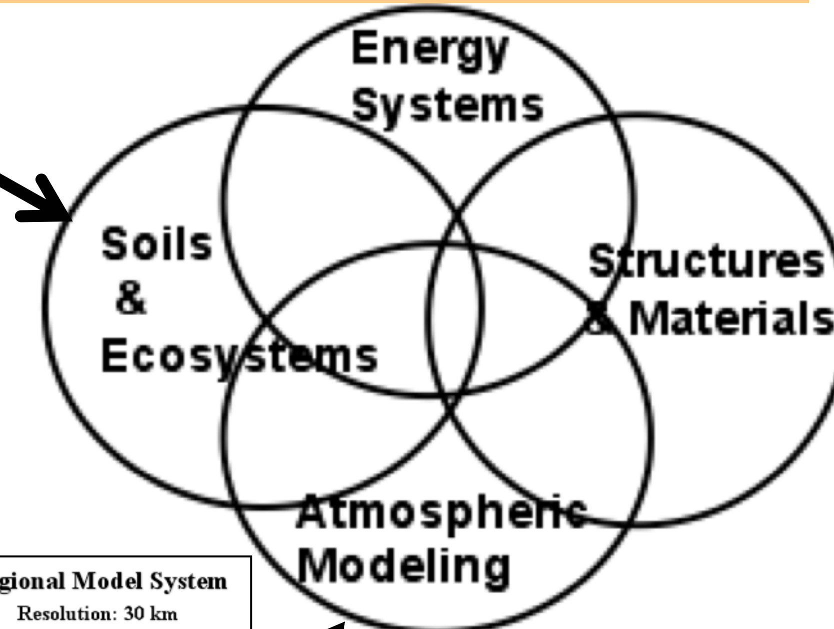
# Milestones FY2008-- LANL

- Global Scenario (2050) -- w/ UIUC
  - Economic $H_2$ penetration & production technology
  - Leak sensitivity studies 1 to 7%
  - IPCC Climate Scenarios ($CO_2$, $N_2O$, $CH_4$ rise)
  - Stratospheric Halocarbon Reduction
  - NOx, Hydrocarbon, CO reduction or redistribution
- Urban Scenario (2050) -- w/ UIUC
  - Baseline $H_2$ in cities with oil transportation (Mexico City)
  - Model City for air quality (EERE input, Albuquerque, Mexico City)
  - Downwind impact of production/ coal gasification facility
- Measurements of Current Leakage at
  - $H_2$ steam $CH_4$ reforming production plant (discussions with Chevron)
  - $H_2$ refueling station (discussions with California)
  - $H_2$ fuel cell devices (fuel cells at LANL)
- Improve soil sink function and ecosystem impacts
  - Laboratory Studies (coord. w/ D. Layzell)
  - Field Studies at Valles Caldera (site prepared)

## Approach: Combine measurements, modeling, and analysis into a comprehensive picture

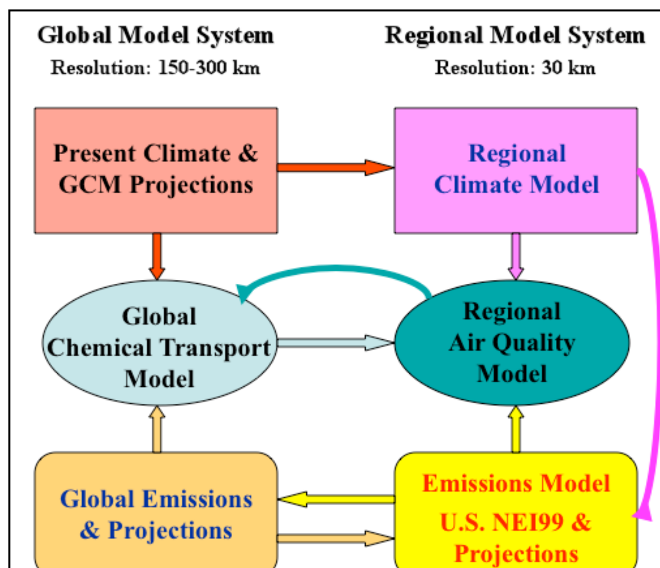



Laboratory and field observations




Energy System Projections and Analysis

Global and Regional Modeling of Air Quality, Ozone Layer, and Climate Effects




H2 Leak Assessment, Sensitivity studies, Analyses of Structures and Materials; Embrittlement

# Accomplishments/ Progress/Results

**We will describe several initial project accomplishments:**

- Development of "worst case" scenario.
- Initial global tropospheric composition model runs.
- Analyses from Mexico City of high urban H2.
- Air quality modeling sensitivity studies
- Soil uptake laboratory studies
- Evaluation of structures and embrittlement issues

# “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 |

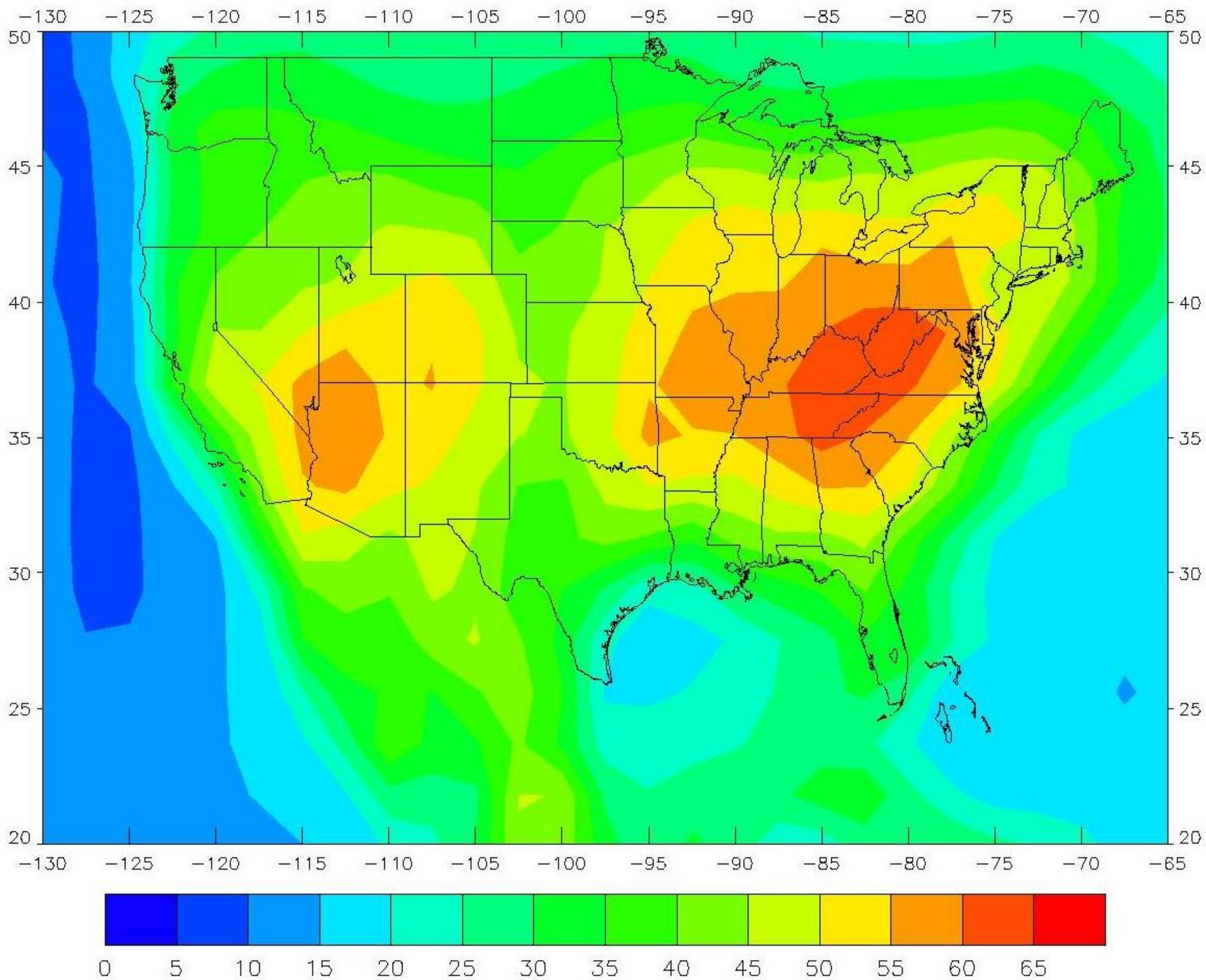
# Model simulated 2050 annual mean global tropospheric burdens of various gases

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

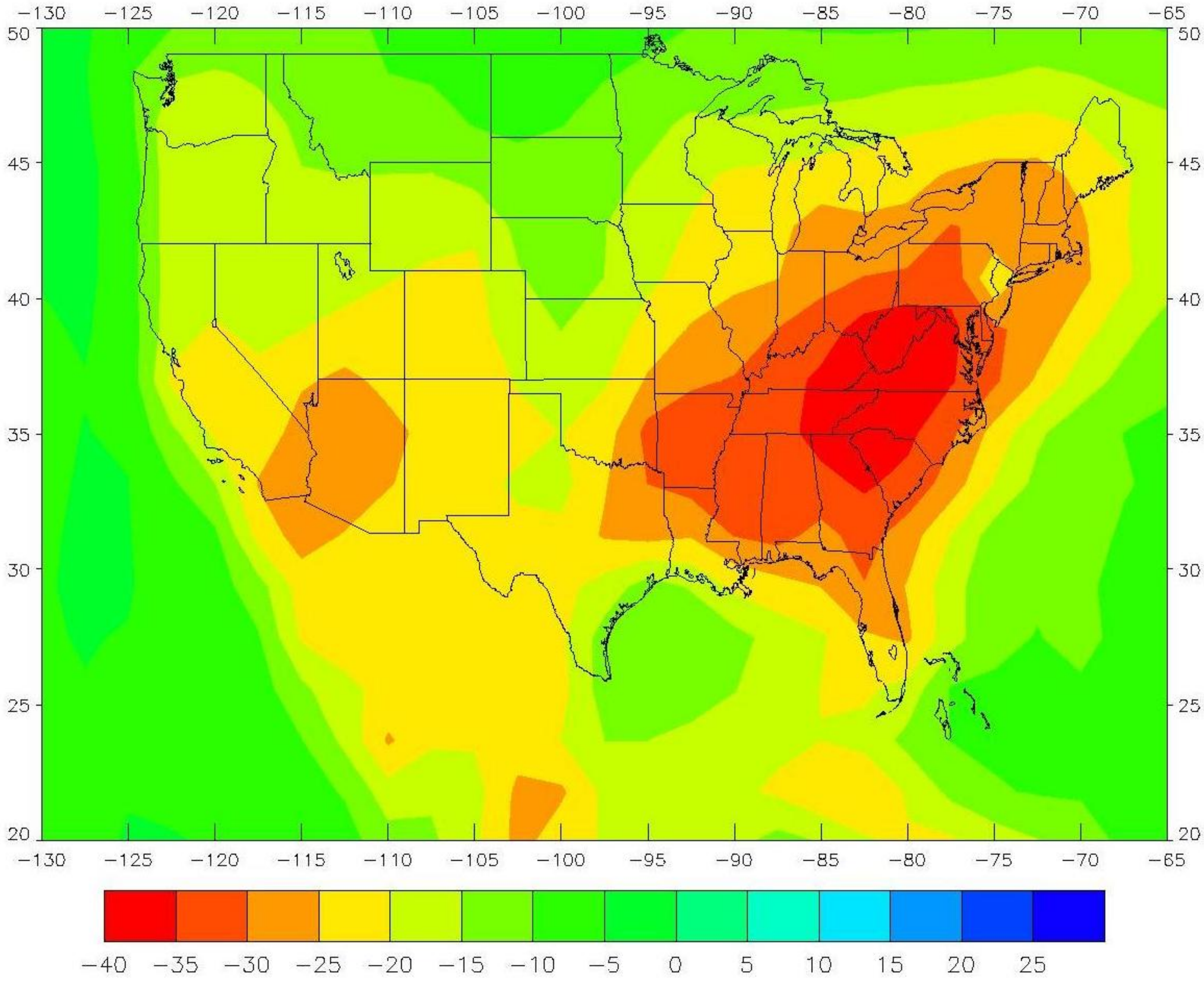
Note: Units are moles

*** It is assumed that under high concentration $H_2$ soil deposition uptake would be 2 times as much as the current value.**

# 2050 contiguous U.S. summer mean surface $O_3$ concentration under IPCC A1FI scenario (in ppb)

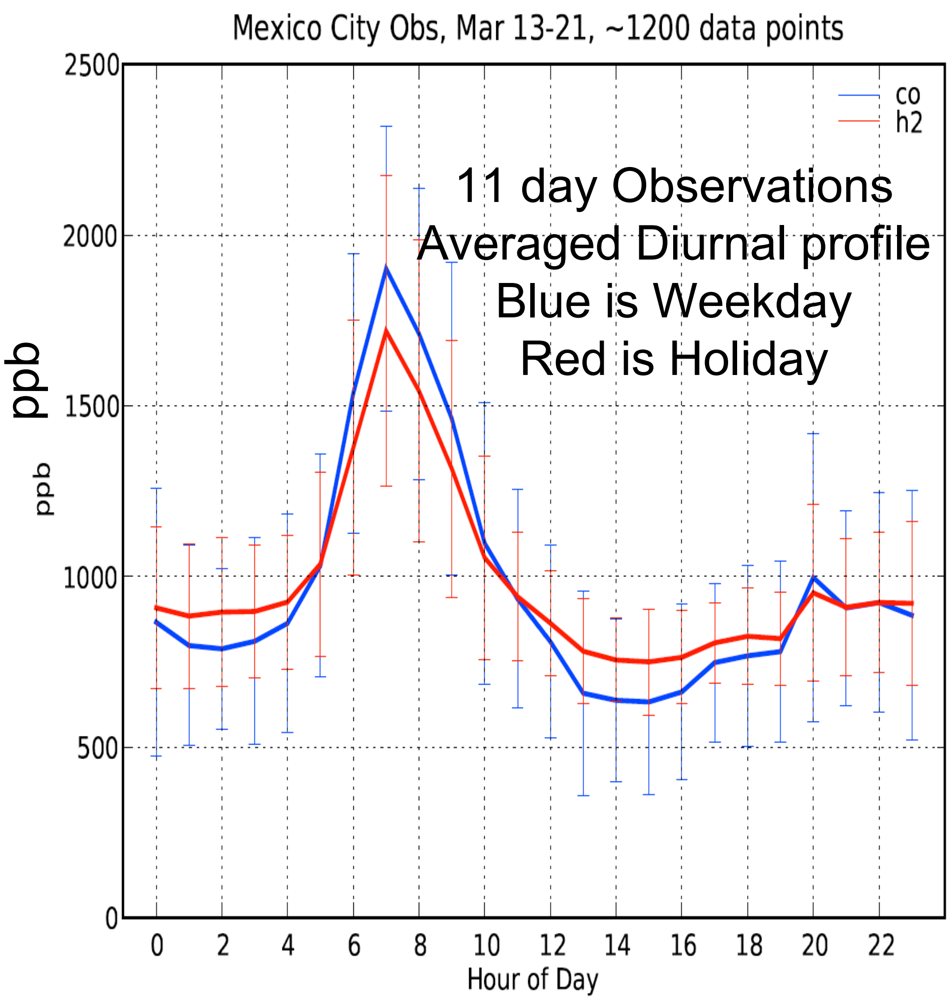


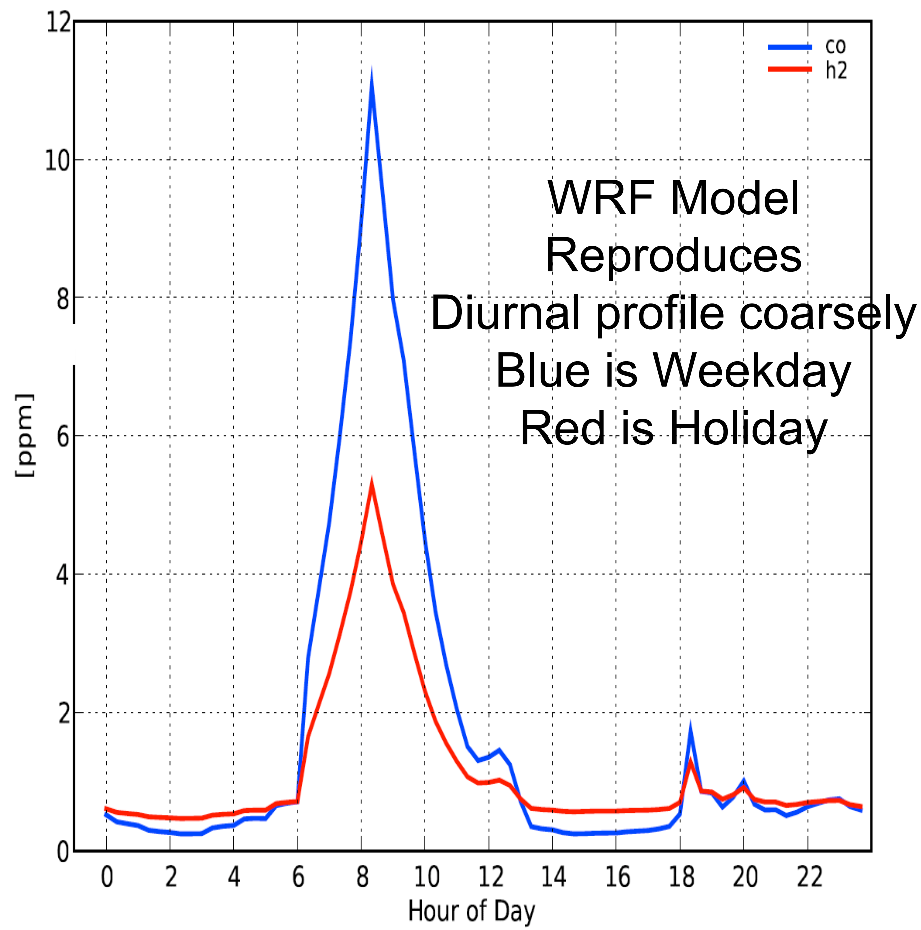
# 2050 hydrogen society contiguous U.S. summer mean surface $O_3$ concentration (with NOx and NMHC reduced and soil uptake adaptation assumption) change with respect to IPCC A1FI scenario (in ppb)



# Regional analyses: What is the $H_2$ baseline in cities from current transportation?

Petrol/diesel cars/trucks emit $H_2$/CO from water-shift ($CO_2$+$H_2$=$H_2O$+ CO) reaction in engine: Record levels of H2 (~5 ppm) measured in Mexico City



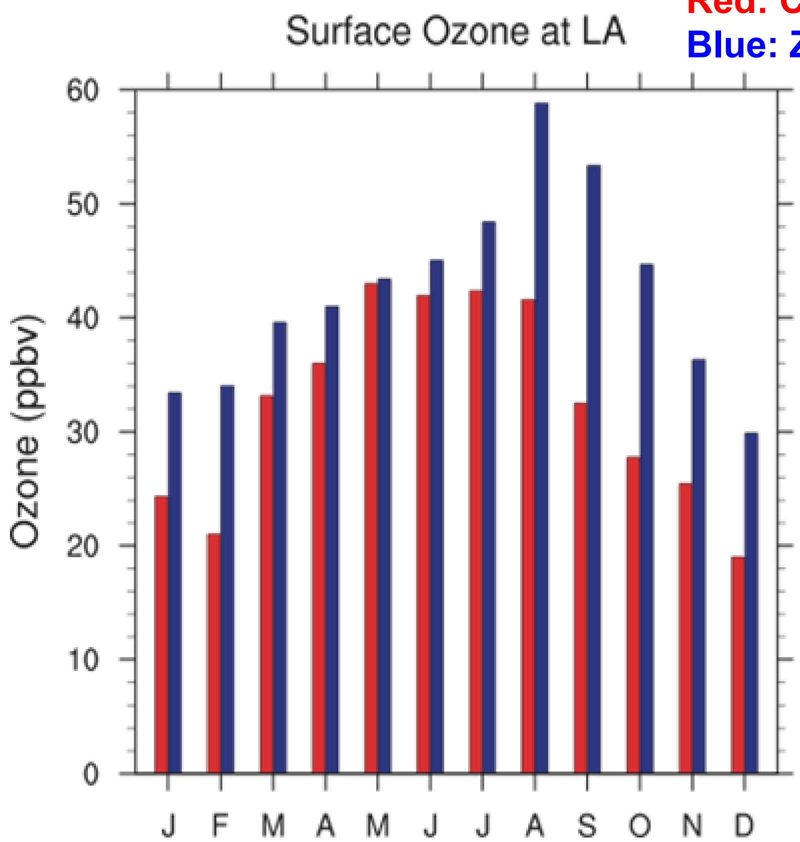

Dubey et al DOE-OBER-funded MILAGRO field campaign

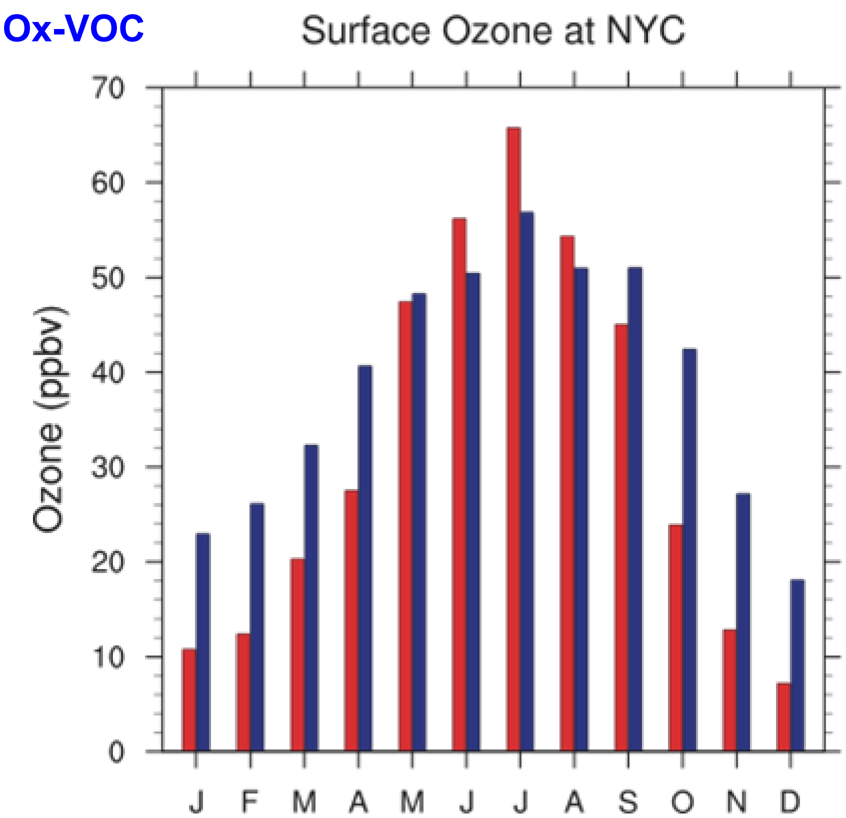
Modeling this project: EERE-OBER synergy

# Surface Ozone Changes for zero VOC and NOx from transportation

Coarse MOZART global simulation results over Los Angeles and New York City

Red: Current NOx-VOC
Blue: Zero NOx-VOC




Increases (VOC limited)

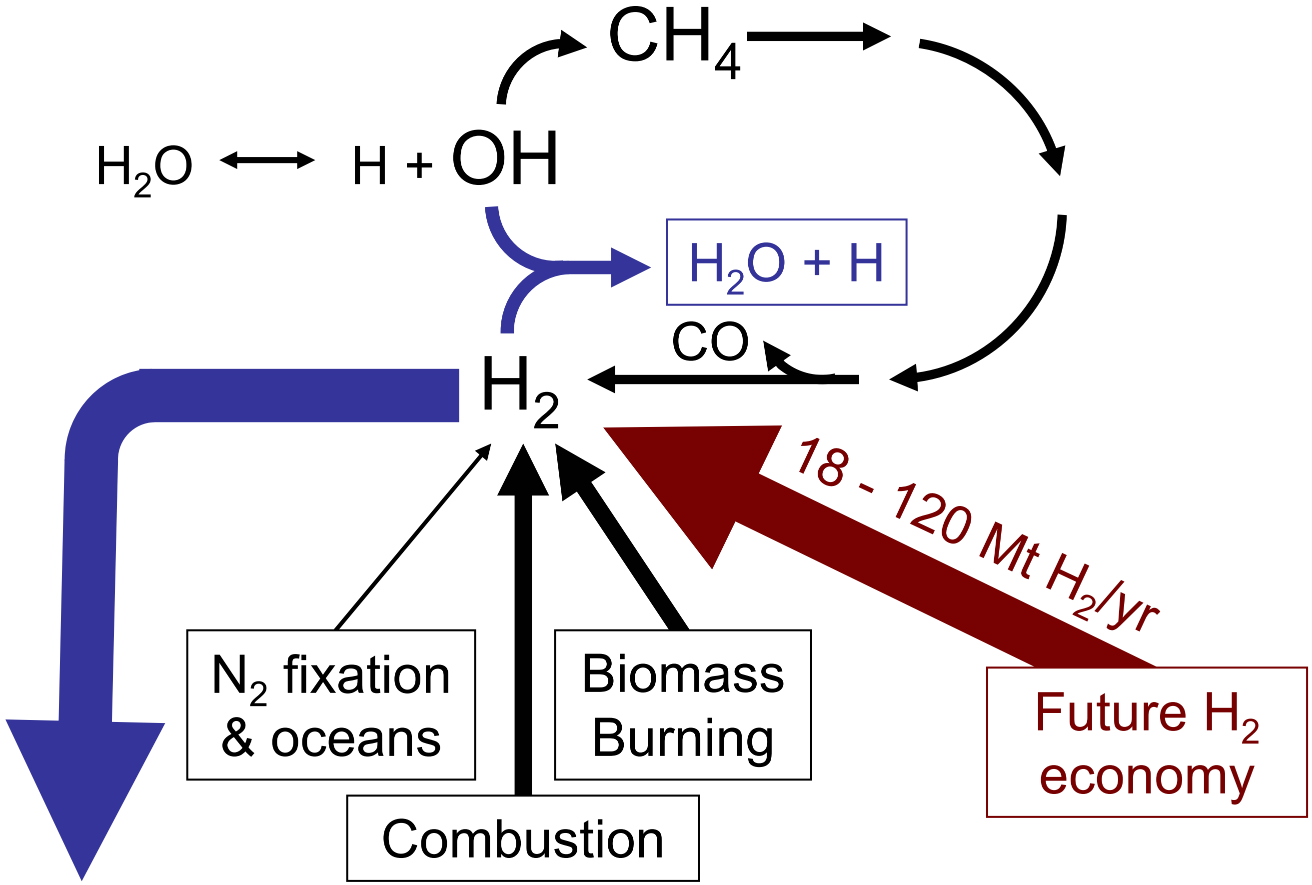
Summer reductions (NOx limited)

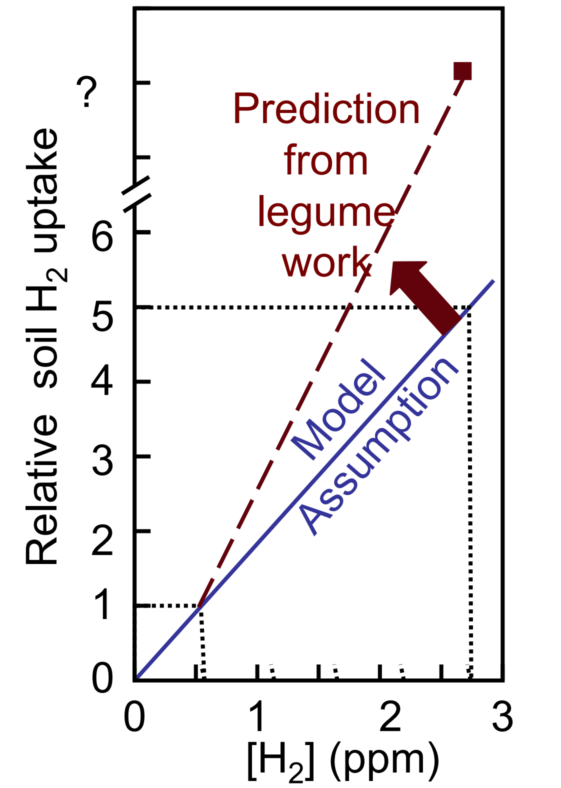
**Background VOC and NOx from other sources, cause different response**

We are refining this urban assessment using regional high resolution models

# The Global $H_2$ Cycle & the Future $H_2$ Economy

**Prediction:** *$H_2$ leaks increases [$H_2$], reduces [OH]; increase $CH_4$ lifetime & force climate change.*



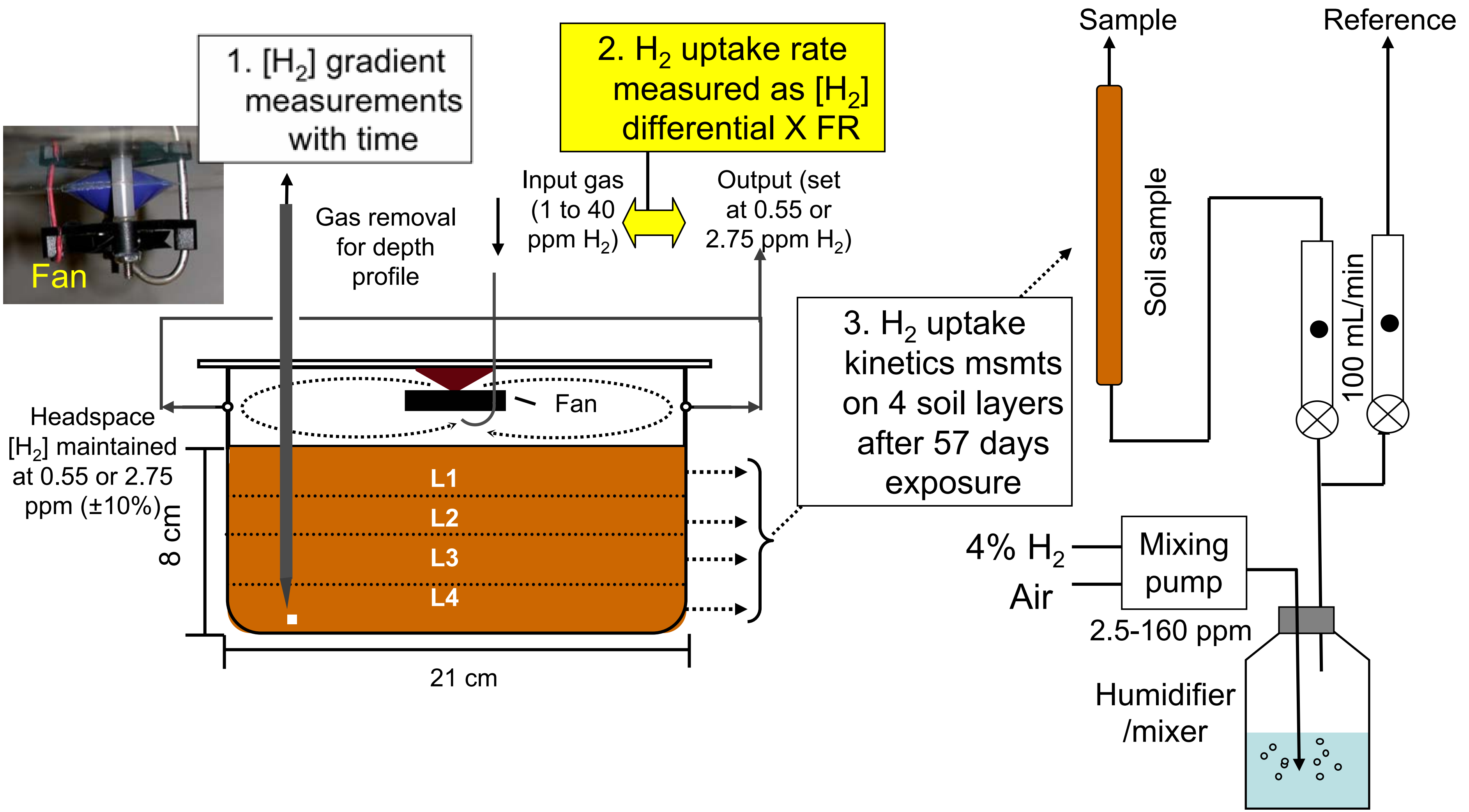




SOILS

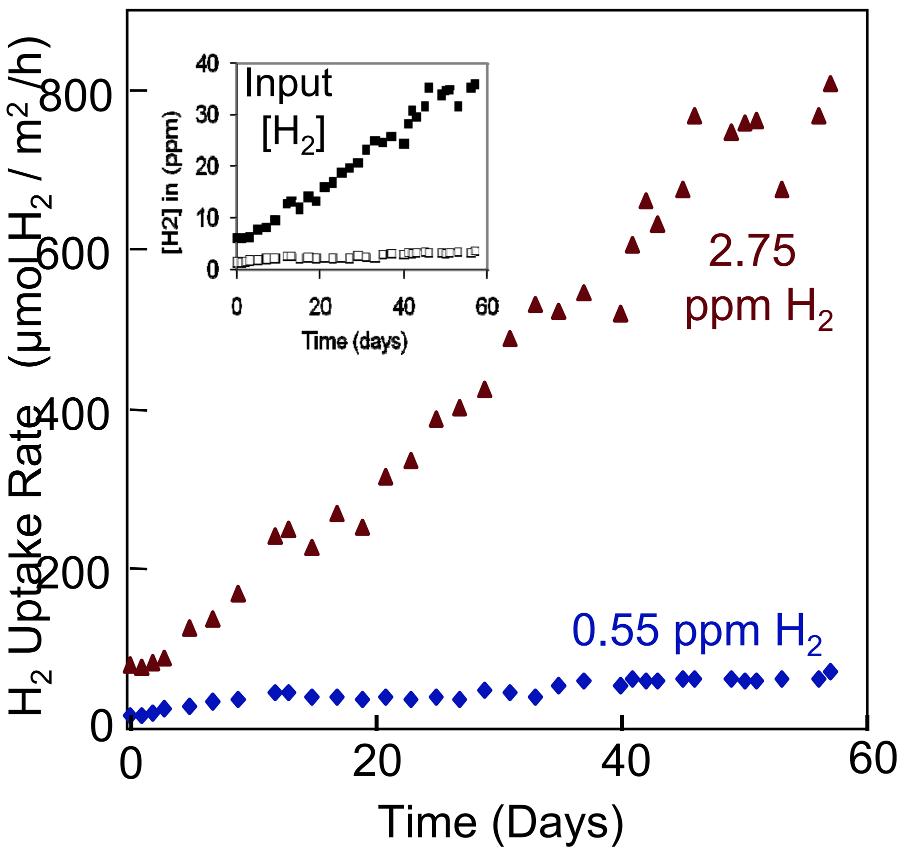
Tromp 2003; Prather 2003; Schultz 2003; Jacobson 2005; Rhee 2006

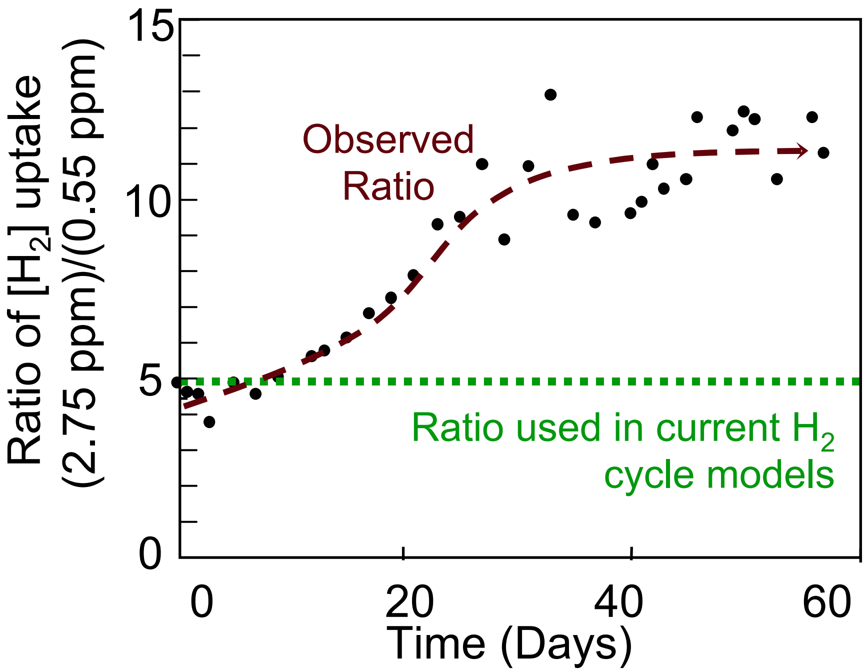
# The Experimental System (Queen's Univ.)

## Determining how soil deposition of $H_2$ changes with time



# **Result:** Net $H_2$ Uptake Increases More at 2.75 ppm $H_2$ than at 0.55 ppm $H_2$



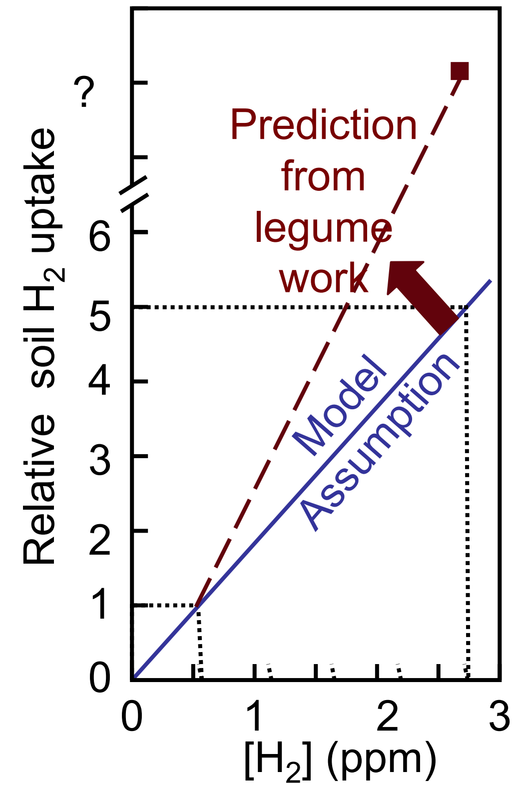




***Conclusion:*** *Model assumptions for $H_2$ deposition rate at elevated $pH_2$ may be underestimated by a factor of 2 or more.*

# Conclusions on Soil Uptake

Soils respond to small (up to 5 fold) increases in atmospheric [$H_2$] by increasing their uptake capacity by more than 5 fold (Range: 8 to 12 fold)?

- *Therefore, previous global $H_2$ cycle 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*



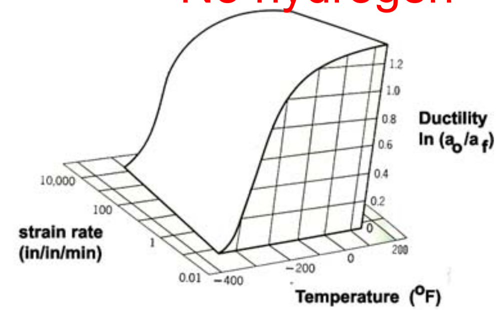

## Further questions

How does vegetation, still air etc affect what [$H_2$] soils actually see? What are the effects of soil drying, heating and cooling on $H_2$ uptake?

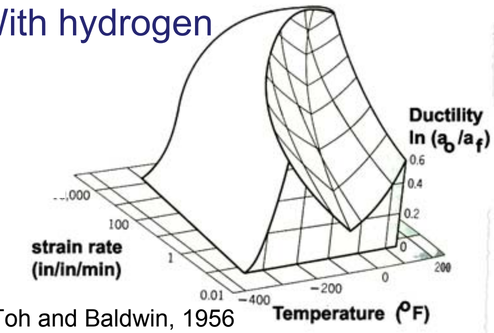
Will a 2 to 5X increase in atmospheric $pH_2$ increase soil fertility *(as it seems to do with a 200 to 500X increase in p[$H_2$] in legume soils)?*

# Hydrogen Embrittlement of Structures

No hydrogen



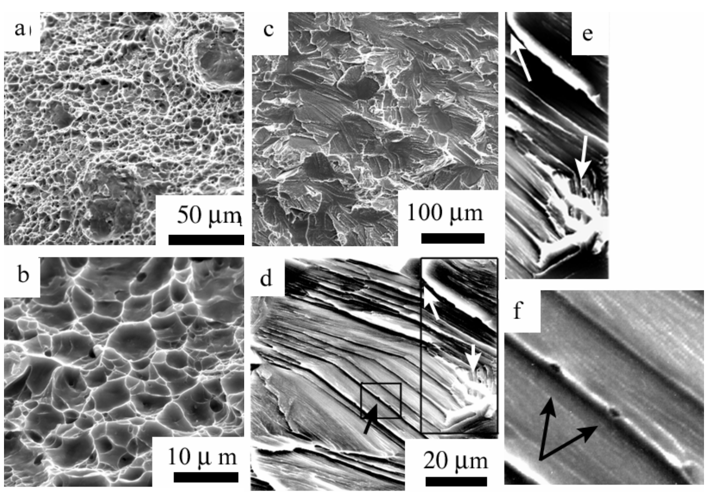

With hydrogen




Toh and Baldwin, 1956

- Surface coatings, including native oxides, should significantly inhibit adsorption and dissociation of $H_2$ and therefore entry of H into the material.
- Constant load conditions prevent disruption of oxide and hydrogen entry to the bulk.
- Hydrogen fugacity and time maintained may be important considerations in developing an internal hydrogen concentration.
- Permeation experiments on structural materials being performed to determine levels.

No hydrogen   With hydrogen




Change in fracture mode

# Future Work

## FY08

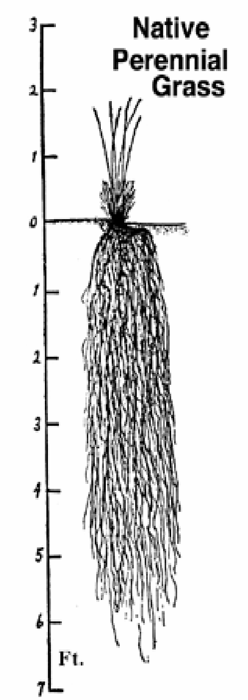
- Complete “worst case” climate and stratospheric modeling studies
- Develop “more realistic” scenarios and evaluate parameter space
- Global chemistry and climate modeling for new scenarios
- Modeling studies to evaluate soil uptake impact
- High resolution urban scale modeling
- Baseline urban H2 emissions from oil transport (extend to US metro: Albuquerque)
- Measure leaks in realistic conditions
- Ecosystem response and soil sink as a function of climate parameters in Valles Caldera
- Initial development of simplified assessment model
- Complete report on materials and structures

## FY09

- Incorporate new soil uptake info into modeling studies
- Complete scenario development and modeling studies
- Complete simplified assessment model

# LANL Experiments in Summer 2008 will explore $H_2$ uptake in the field to verify laboratory studies

VALLES CALDERA
NATIONAL PRESERVE

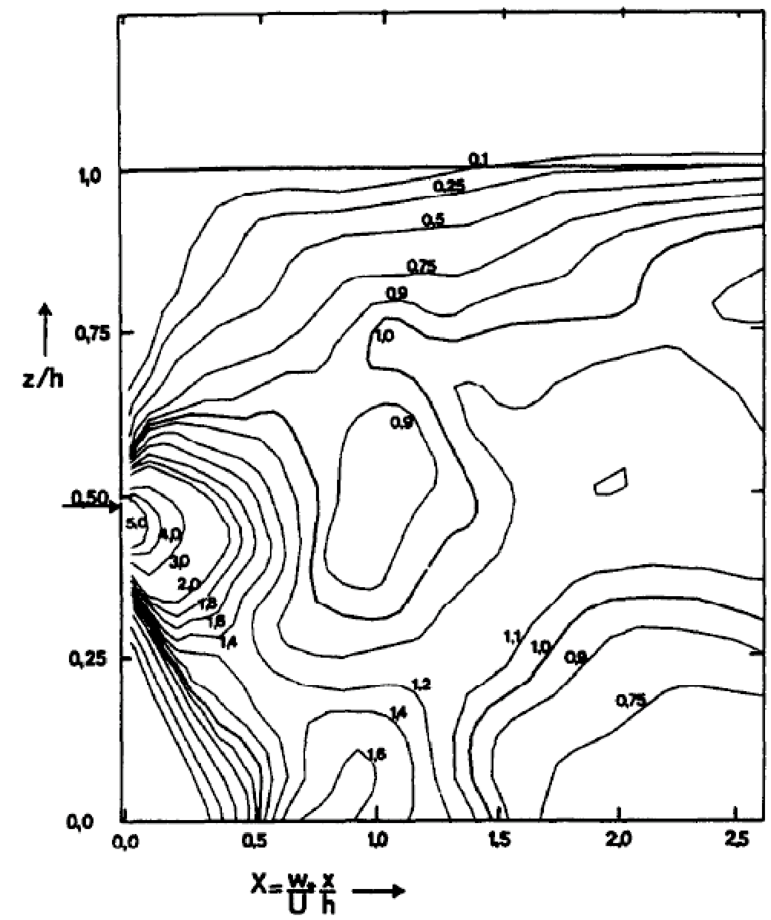




Grassland field site where summer in situ measurements will be performed. Current analyses include continuous meteorology, carbon, water and sensible heat fluxes, soil temperature and moisture, incoming and outgoing long and shortwave radiation, etc. Chamber and profile measurements will determine $H_2$ uptake.

# Future Work – Oxygen Plumes

- Analysis of oxygen plumes as a local risk for fire or other changes will be based on earlier plume calculations for point sources.
- Scale the results for hydrogen production source flux.
- Determine range at which a plume would have a dangerous oxygen content.




Sample plume calculation from F.T. M. Nieuwstadt and J.P.J.M.M. de Valk, *Atmospheric Environment*, v. 21(12) pp. 2573-2587 (1987).

# Summary

**In first 6 months of the project:**

- **Initial scenario development – "worst case" scenario towards determining maximum possible effects on ozone, hydroxyl, aerosols, climate**
- **Resulting global model study**
  - **Air quality issues (ozone, PM) decrease dramatically**
  - **Global hydroxyl (OH) effects**
  - **Global troposheric ozone**
- **Regional modeling studies started**
- **Long-time scale laboratory studies suggest 2x previous estimates of $H_2$ uptake rate in soils**
- **Atmospheric $H_2$ Effects on structures and embrittlement not likely to be important**