DOE Hydrogen Program

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

Don Wuebbles

University of Illinois at Urbana-Champaign

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AN13

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

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

Barriers

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

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)

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

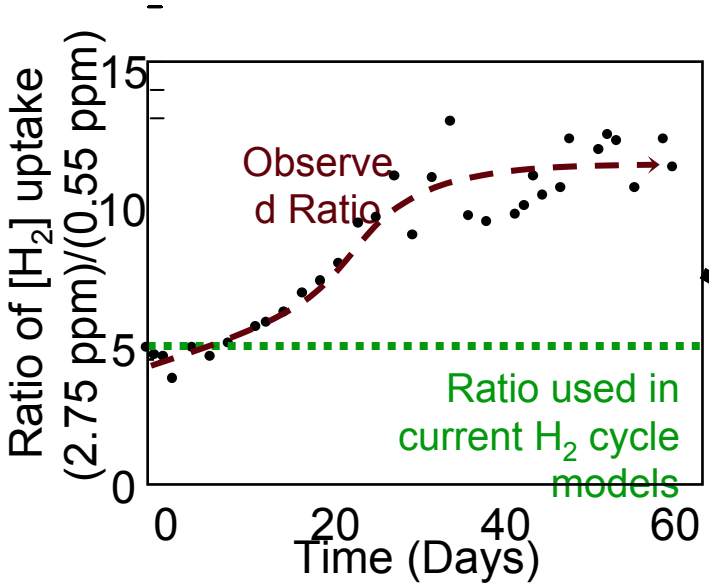
- **Evaluate criteria pollutants emitted from distributed and centralized hydrogen production pathways**
- **Evaluate criteria pollutants emitted for different scenarios of vehicle market penetration**
- **Determine impact of hydrogen releases on the oxidative capacity of the atmosphere.**
- **Determine 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

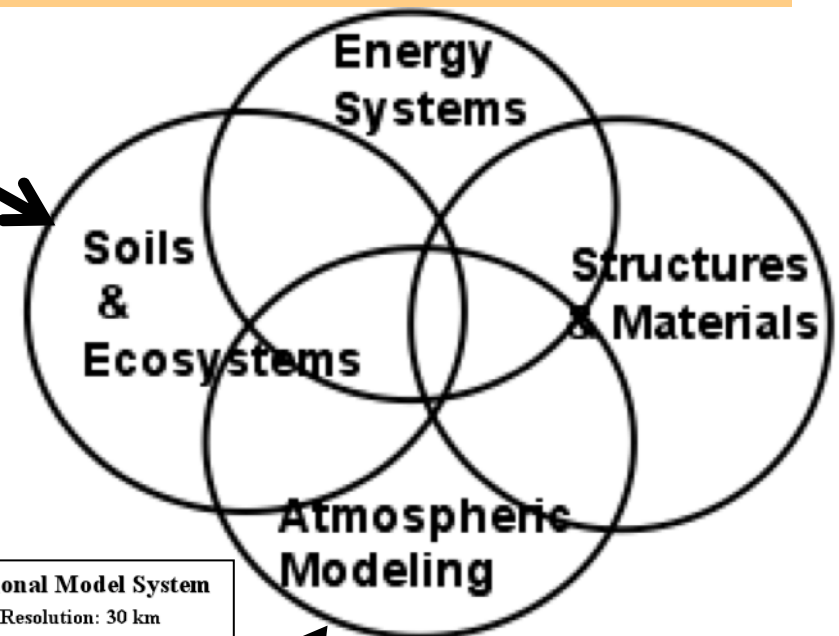
- **Establish criteria for initial scenario development**
- **Identify and develop U.S. and global scenarios using energy system model.**
- **Assess displaced emissions effects for selected scenarios**
- **With developed scenarios, design the atmospheric model calculations to assess global chemistry 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)

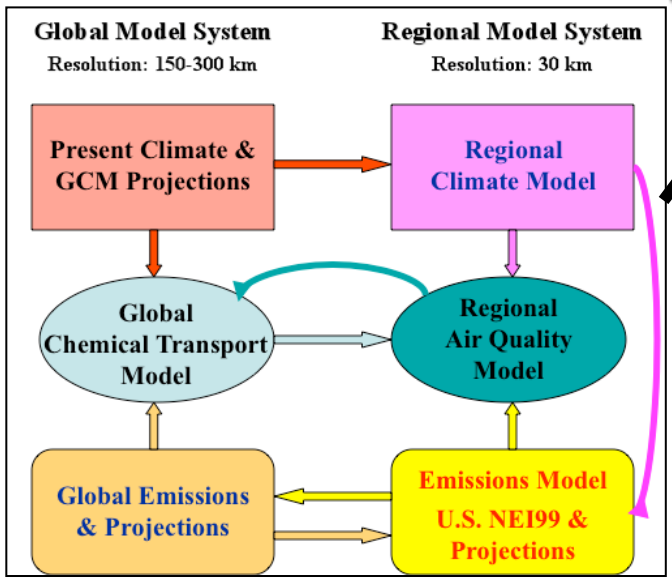


Approach: Combine measurements, modeling, and analysis into a comprehensive picture



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

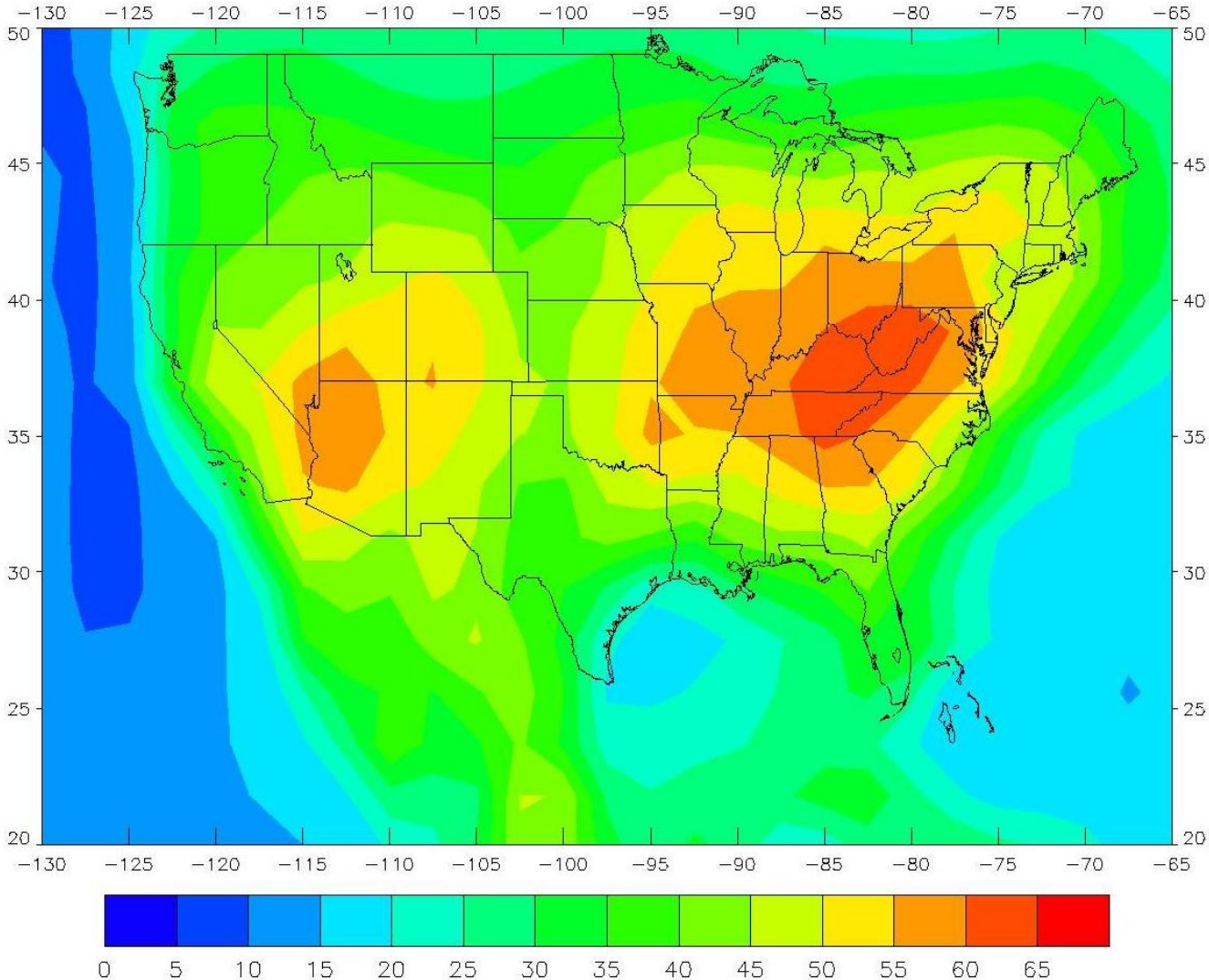
Model simulated 2050 annual mean global tropospheric burdens of various gases

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

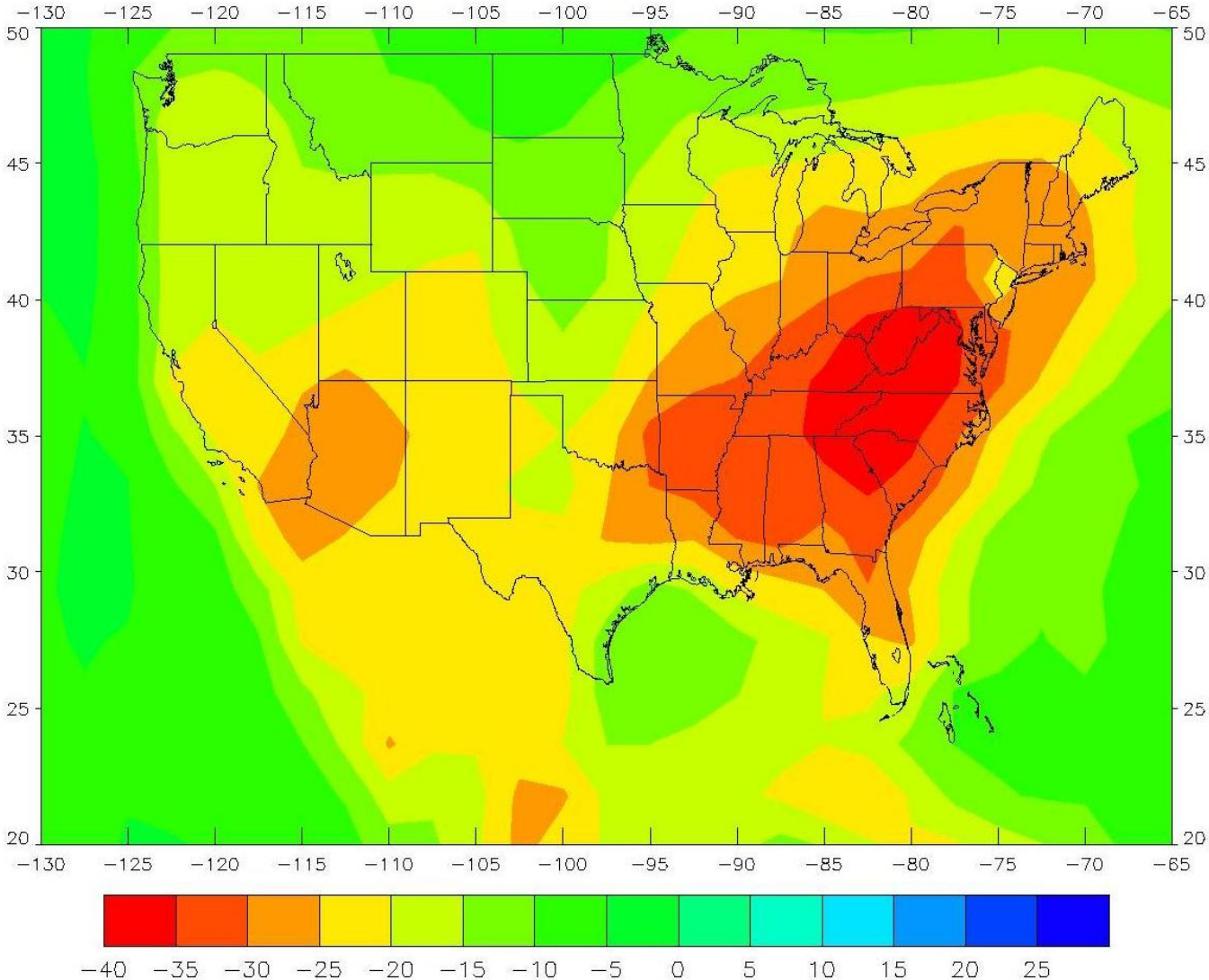
Note: Units are moles

*** 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)

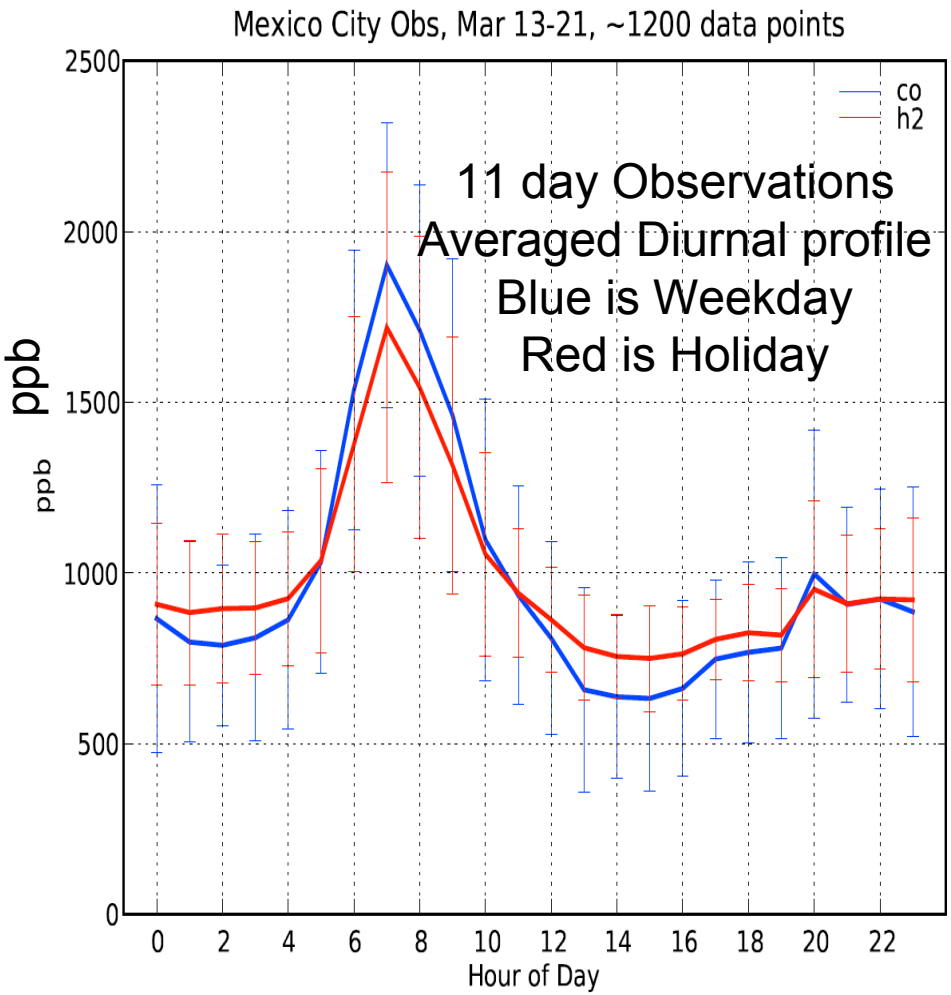


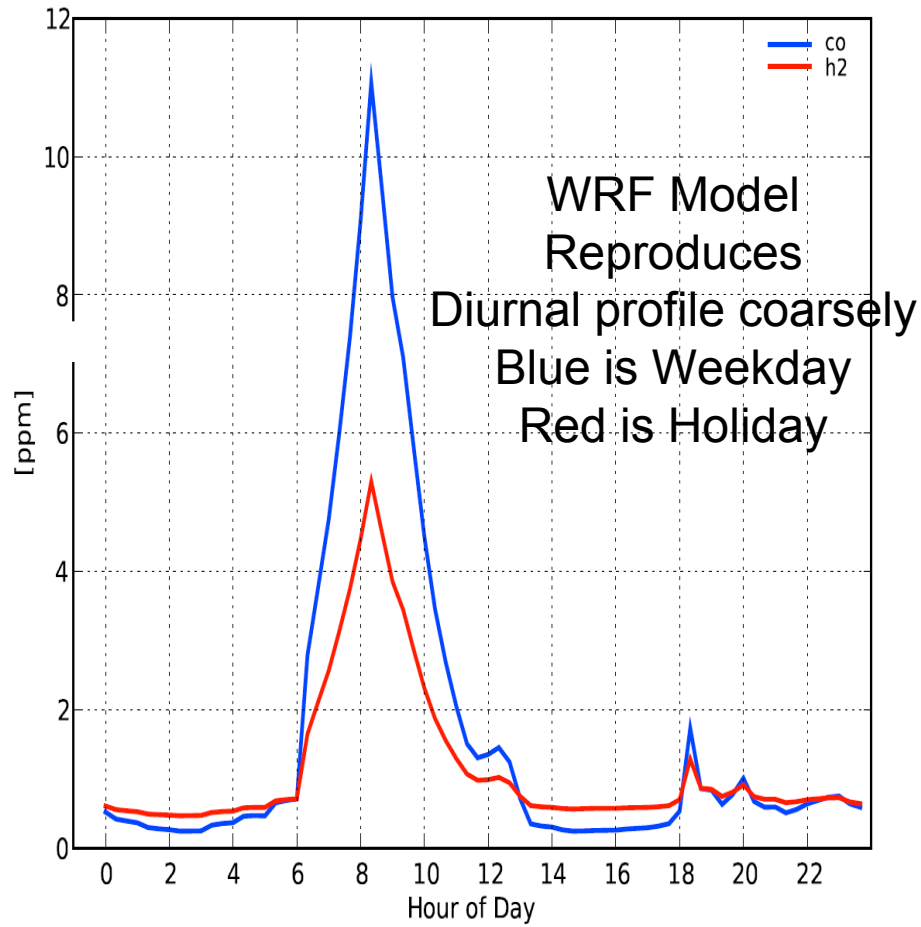
2050 hydrogen society contiguous U.S. summer mean surface O_3 concentration (with NOx and NMHC reduced and soil uptake adaptation assumption) change with respect to IPCC A1FI scenario (in ppb)



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





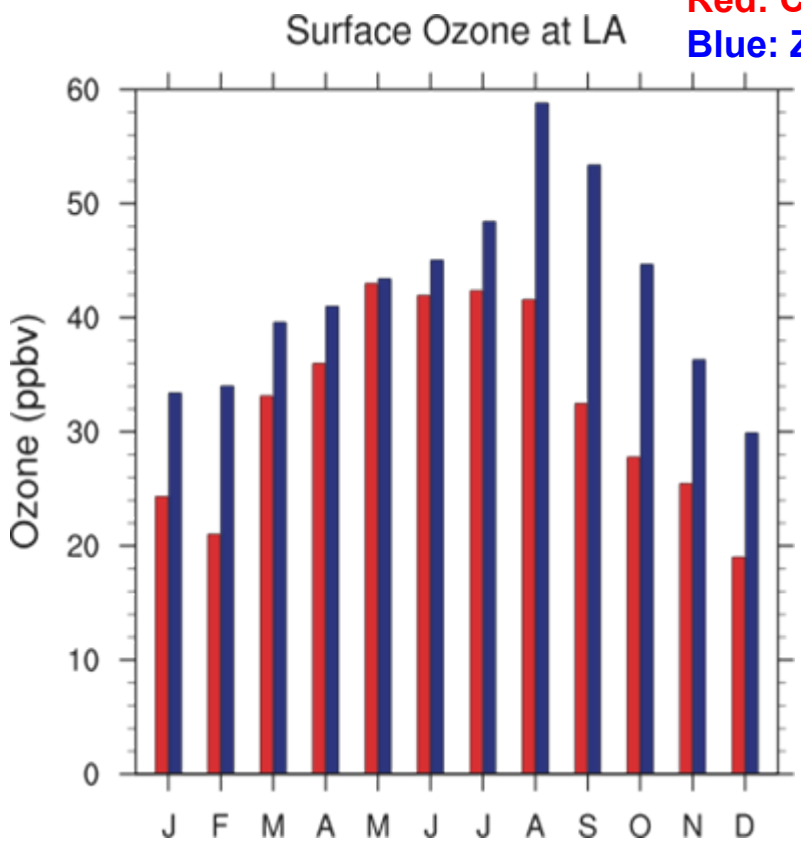
Dubey et al DOE-OBER-funded MILAGRO field campaign

Modeling this project: EERE-OBER synergy

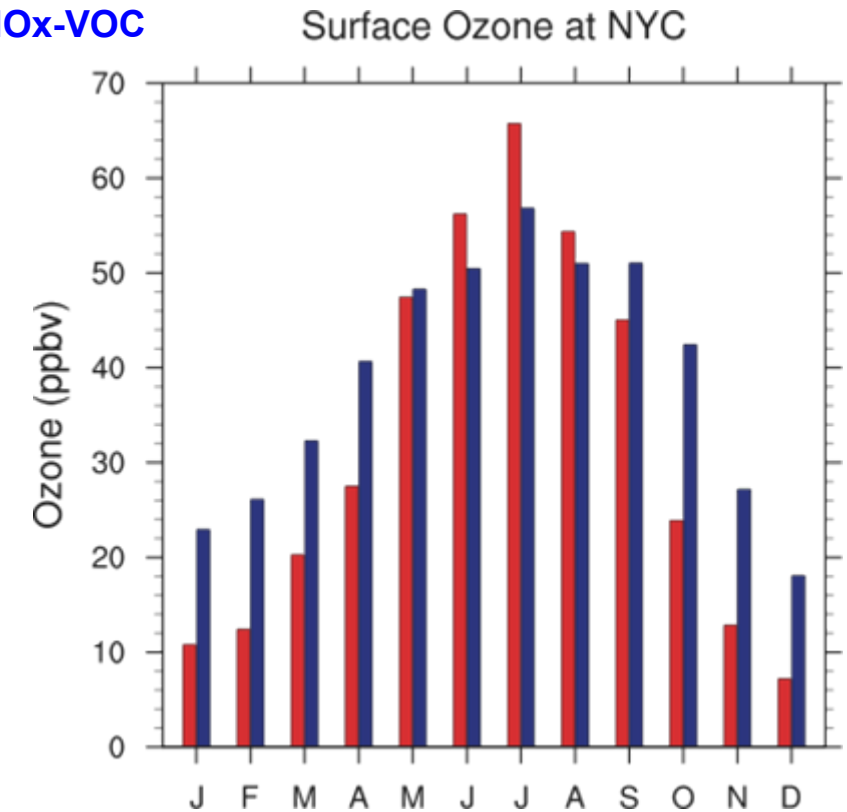
Surface Ozone Changes for zero VOC and NOx from transportation

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

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



Increases (VOC limited)



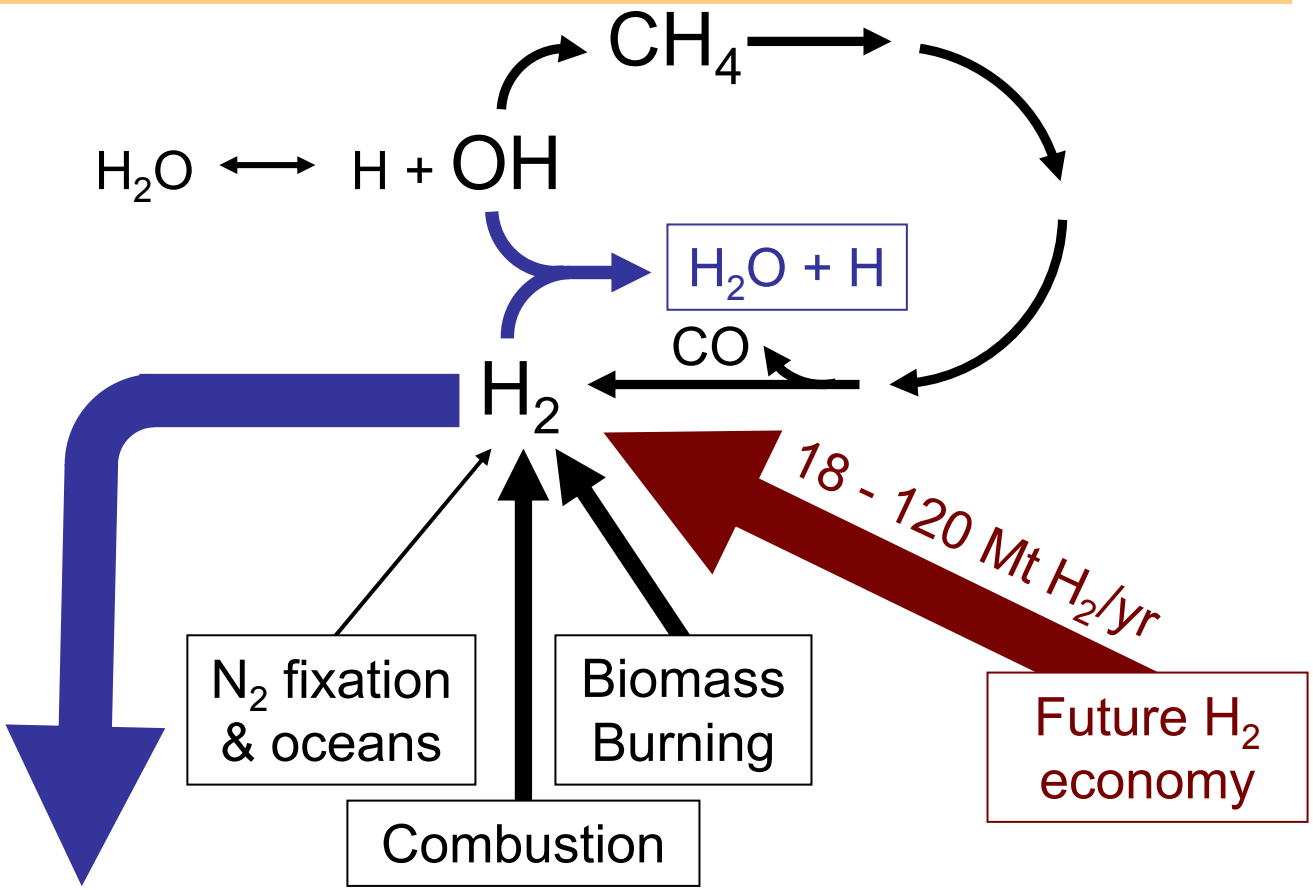
Summer reductions (NOx limited)

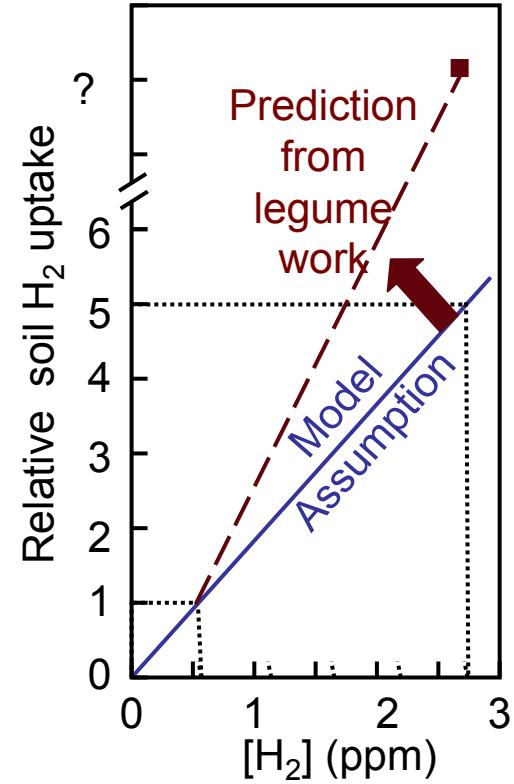
Background VOC and NOx from other sources, cause different response

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.*



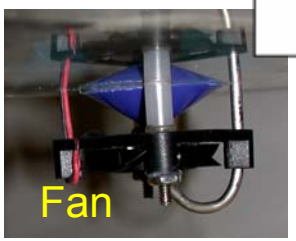


SOILS

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



1. $[H_2]$ gradient measurements with time

2. H_2 uptake rate measured as $[H_2]$ differential X FR

3. H_2 uptake kinetics msmts on 4 soil layers after 57 days exposure

Gas removal for depth profile

Input gas (1 to 40 ppm H_2)

Output (set at 0.55 or 2.75 ppm H_2)

Fan

Headspace $[H_2]$ maintained at 0.55 or 2.75 ppm (±10%)

8 cm

L1

L2

L3

L4

21 cm

Sample

Reference

Soil sample

100 mL/min

4% H_2

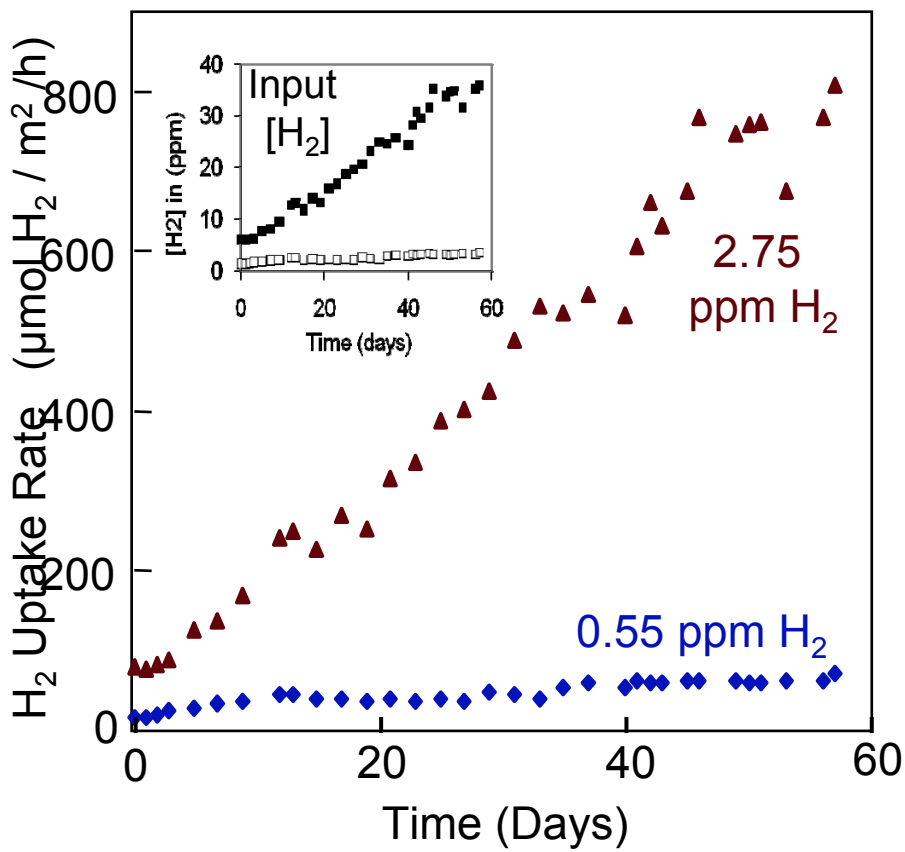
Air

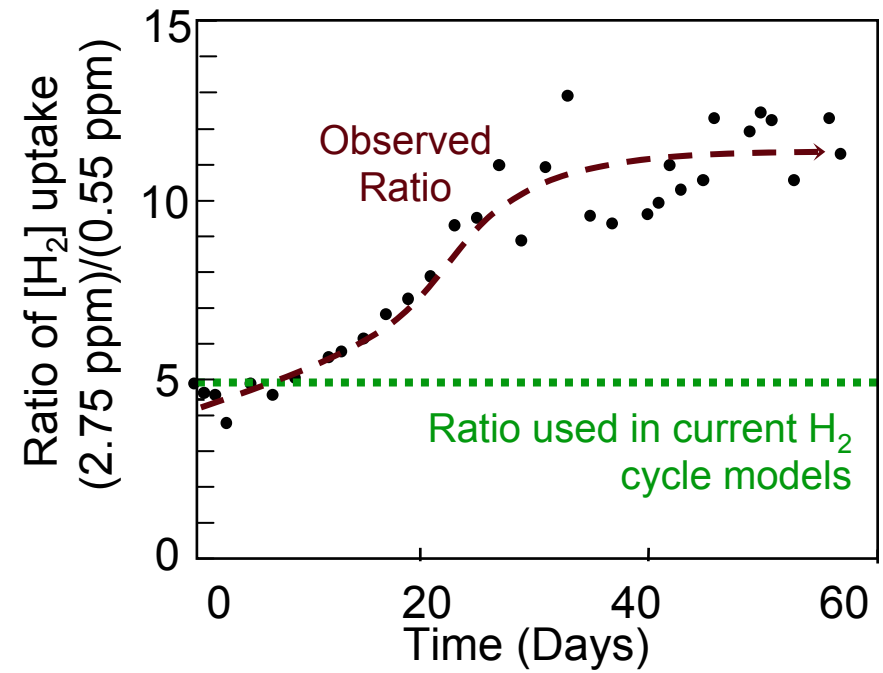
Mixing pump

2.5-160 ppm

Humidifier /mixer

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



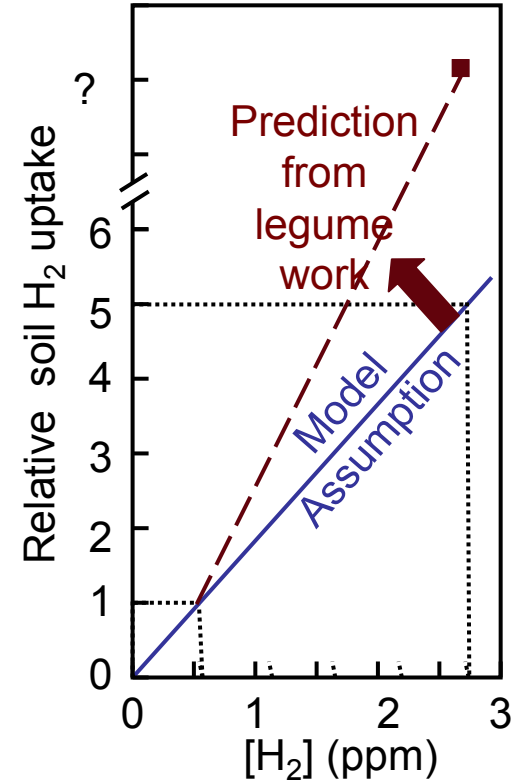


Conclusion: *Model assumptions for H_2 deposition rate at elevated pH_2 may be underestimated by a factor of 2 or more.*

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

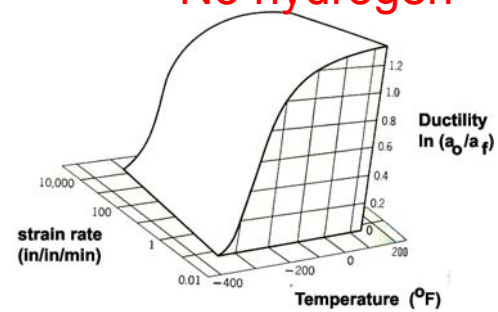
How does vegetation, still air etc affect what [H_2] soils actually see? What are the effects of soil drying, heating and cooling on H_2 uptake?

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)?*

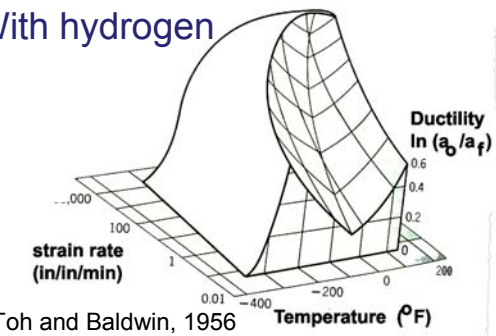
Hydrogen Embrittlement of Structures

- 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

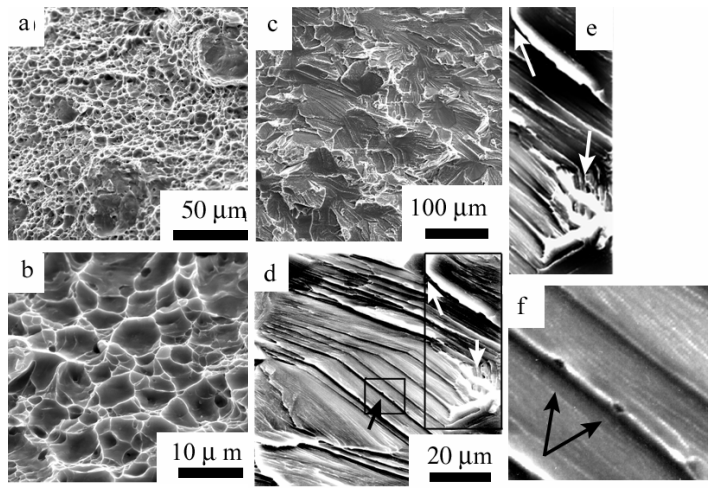


With hydrogen



Toh and Baldwin, 1956

No hydrogen With hydrogen



Change in fracture mode

Future Work

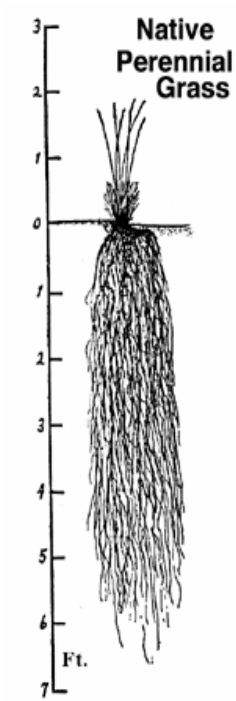
FY08

- 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

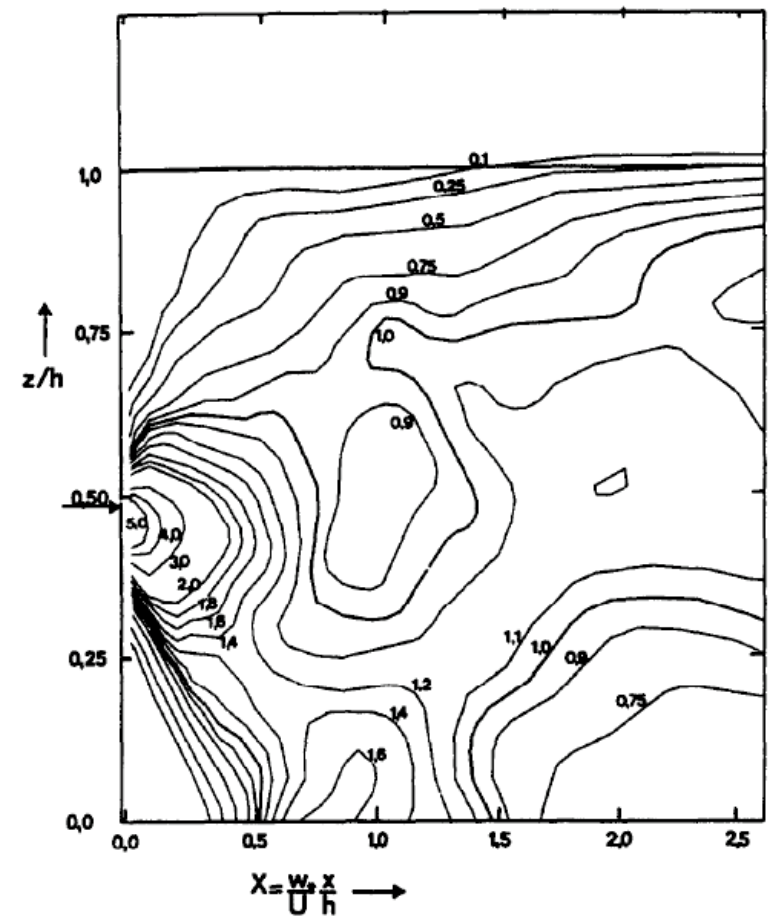
LANL Experiments in Summer 2008 will explore H_2 uptake in the field to verify laboratory studies



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**