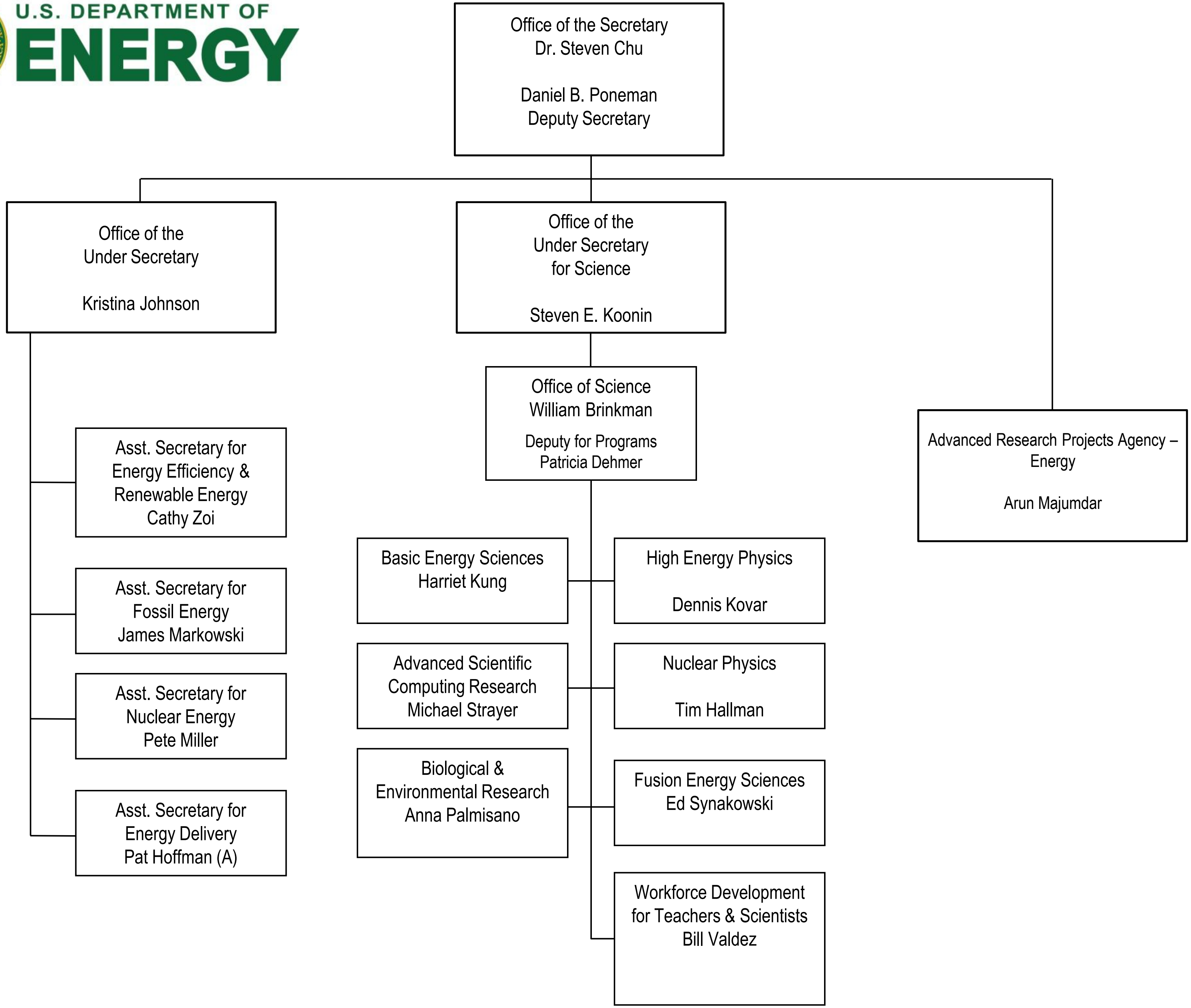
U.S. DEPARTMENT OF ENERGY | Office of Science

Carbon Capture: Beyond 2020

Dr. William F. Brinkman, Director
Office of Science
U.S. Department of Energy

March 4, 2010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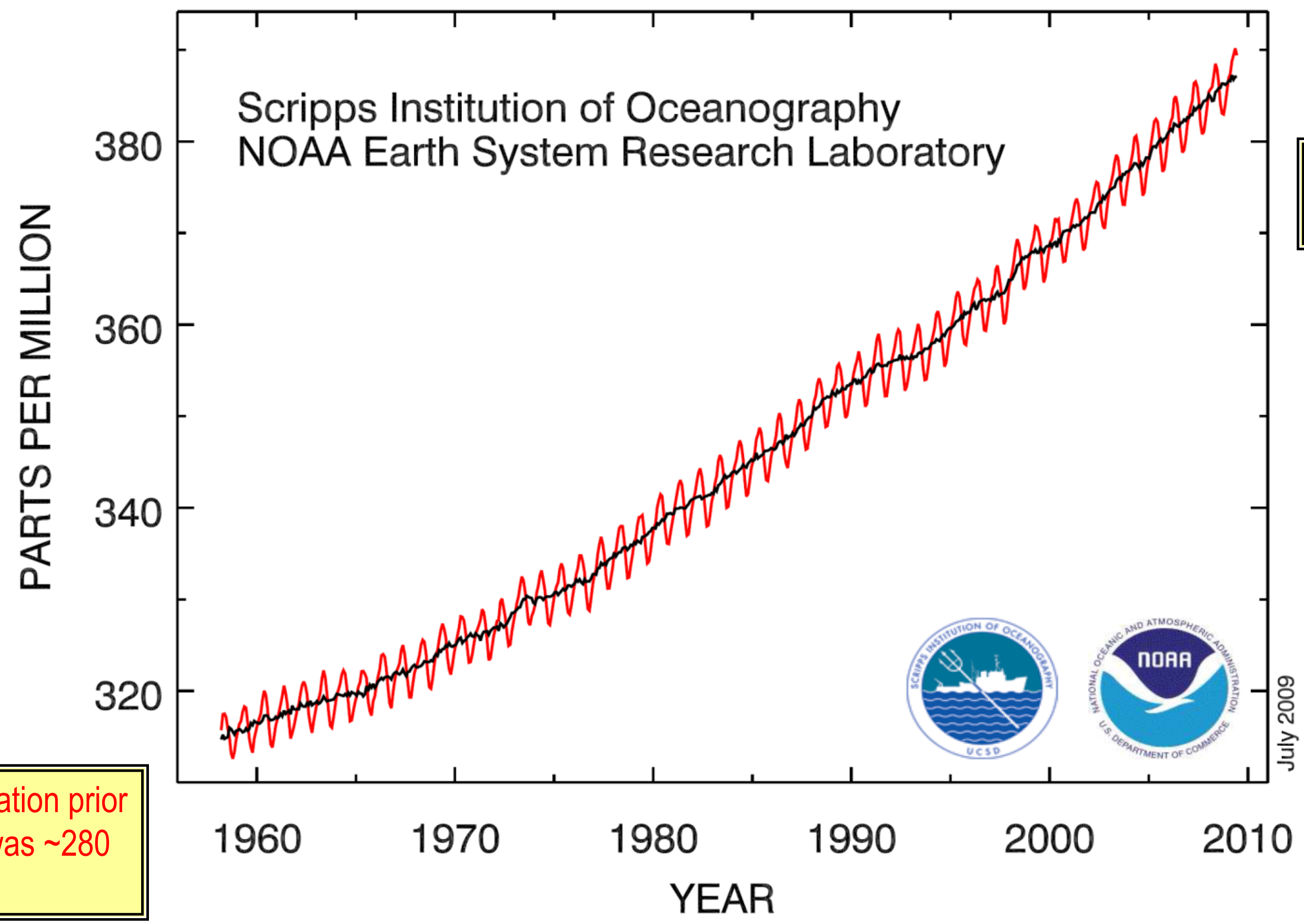
Modern CO_2 Concentrations are Increasing

The current concentration is the highest in 800,000 years, as determined by ice core data

Atmospheric CO_2 at Mauna Loa Observatory



Concentration now ~388 ppm

Concentration prior to 1800 was ~280 ppm

Greenland Ice Mass Loss – 2002 to 2009

Increasing rates of ice mass loss from the Greenland and Antarctic ice sheets revealed by GRACE (Gravity Recovery and Climate Experiment) satellite:

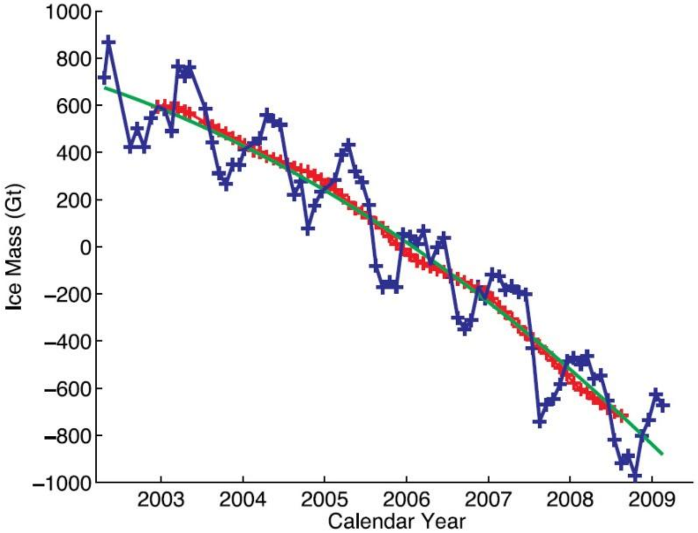
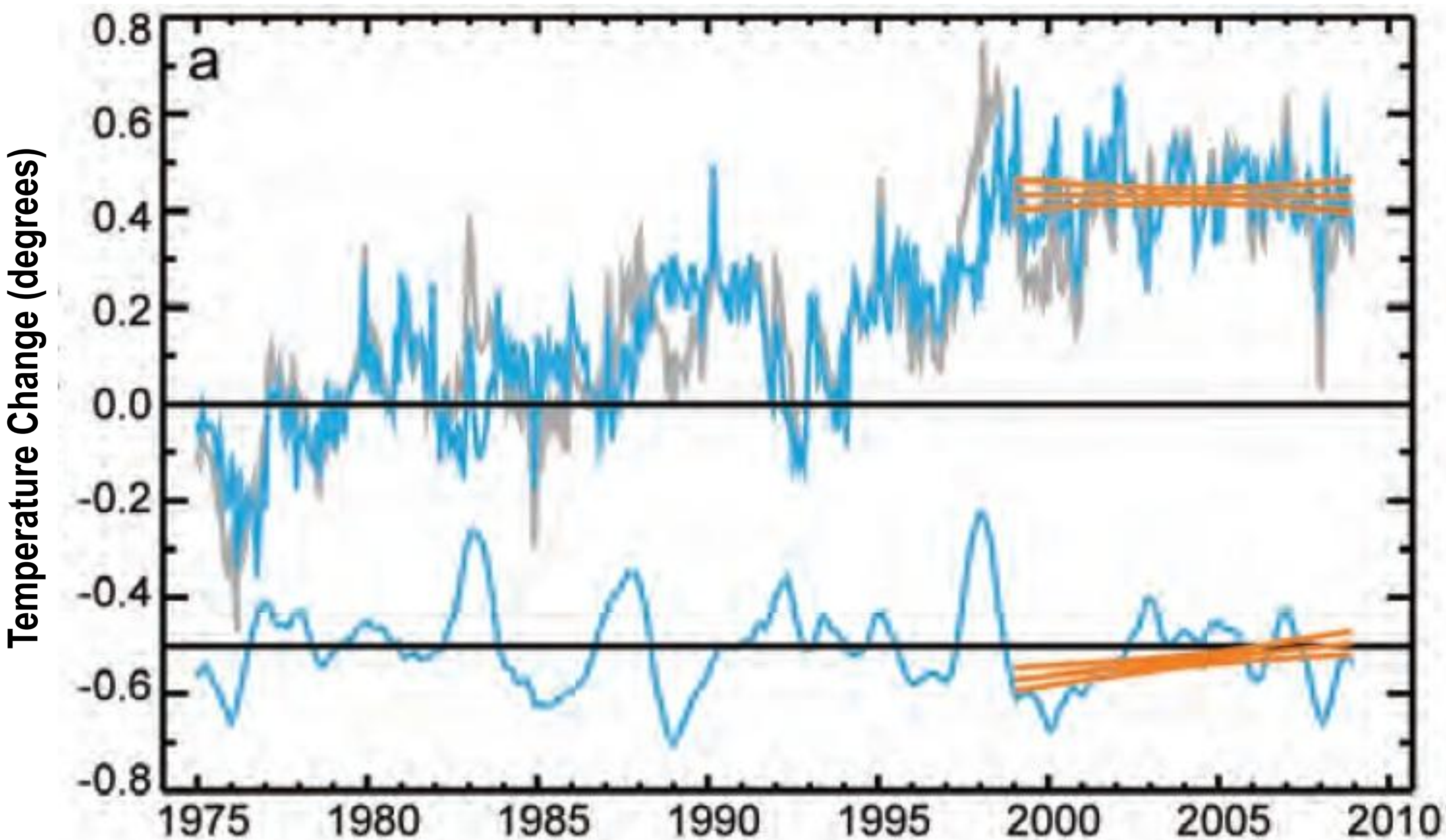


Figure 1. Time series of ice mass changes for the Greenland ice sheet estimated from GRACE monthly mass solutions for the period from April 2002 to February 2009. Unfiltered data are blue crosses. Data filtered for the seasonal dependence using a 13-month window are shown as red crosses. The best-fitting quadratic trend is shown (green line). The GRACE data have been corrected for leakage and GIA.

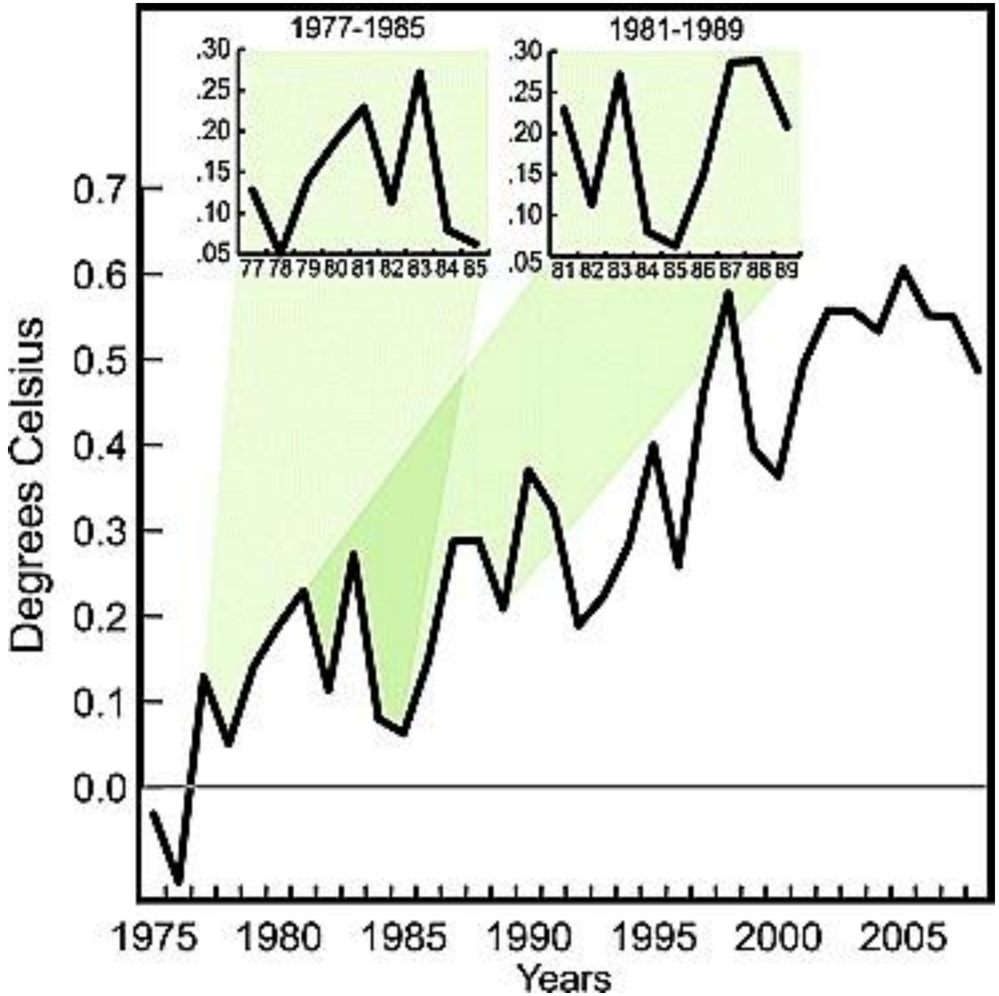
- In Greenland, the mass loss increased from 137 Gt/yr in 2002–2003 to 286 Gt/yr in 2007–2009
- In Antarctica, the mass loss increased from 104 Gt/yr in 2002–2006 to 246 Gt/yr in 2006–2009

I. Velicogna, GEOPHYSICAL RESEARCH LETTERS, VOL. 36, L19503, doi:10.1029/2009GL040222, 2009

Accounting for Stagnation of Global Average Temperature: The Role of Climate Model Variability

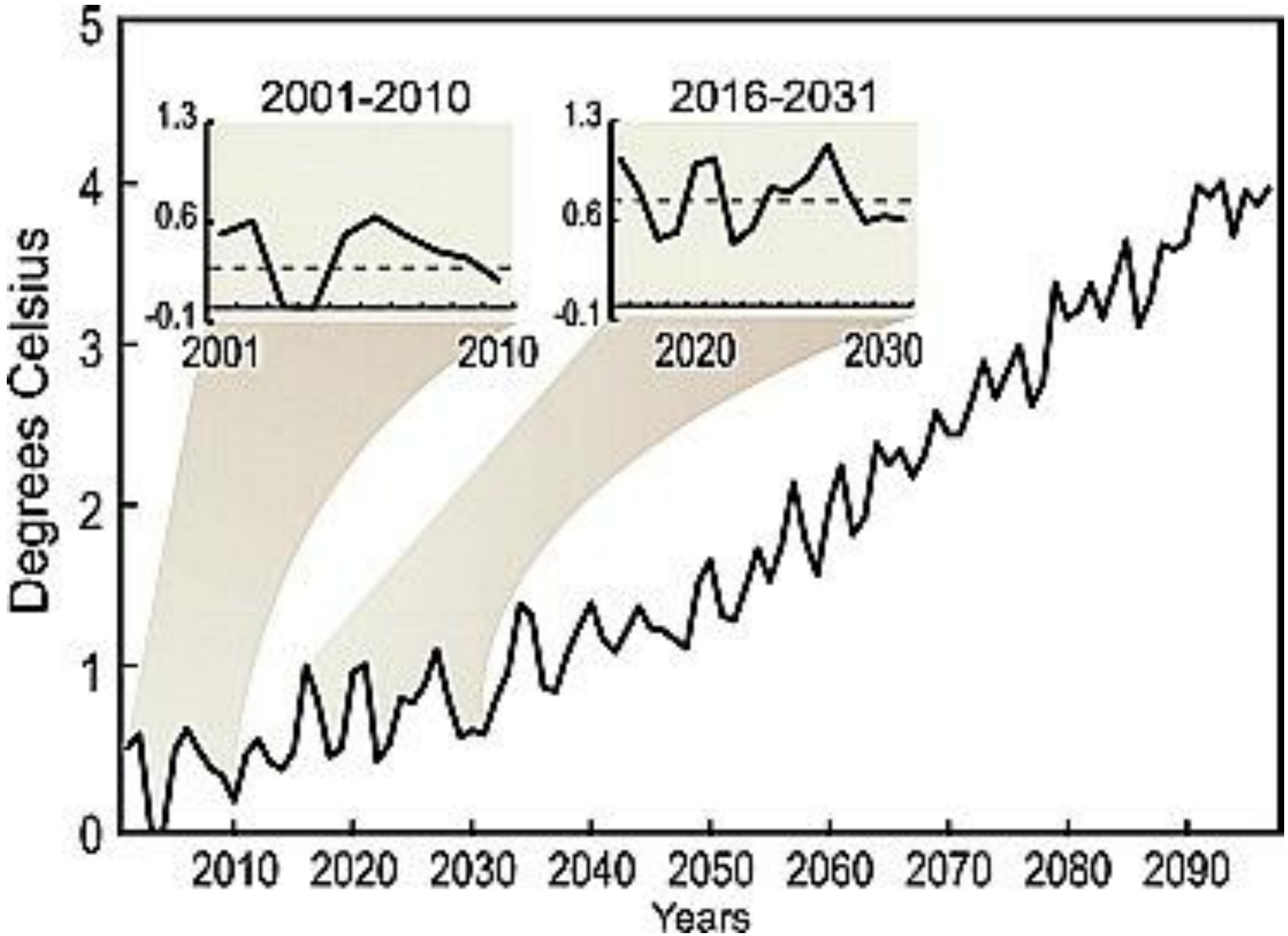


One Realization of the Globally Averaged Surface Air Temperature for Land and Ocean

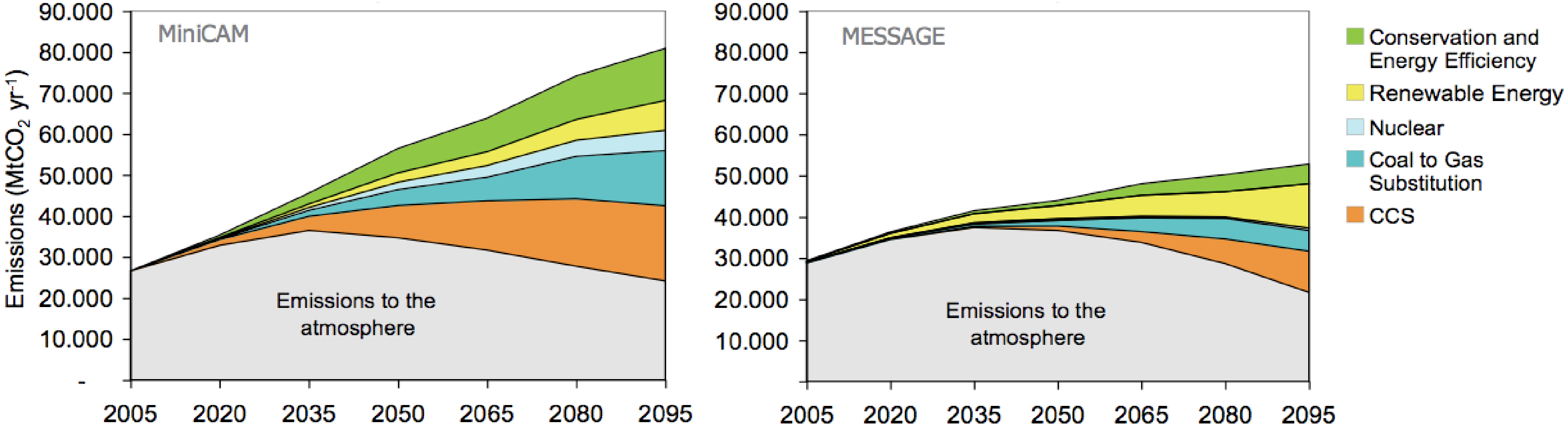


Easterling and Wehner. *Geophysical Research Letters* 36, no. 8 (4, 2009).

A Second Realization of the Globally Averaged Surface Air Temperature for Land and Ocean



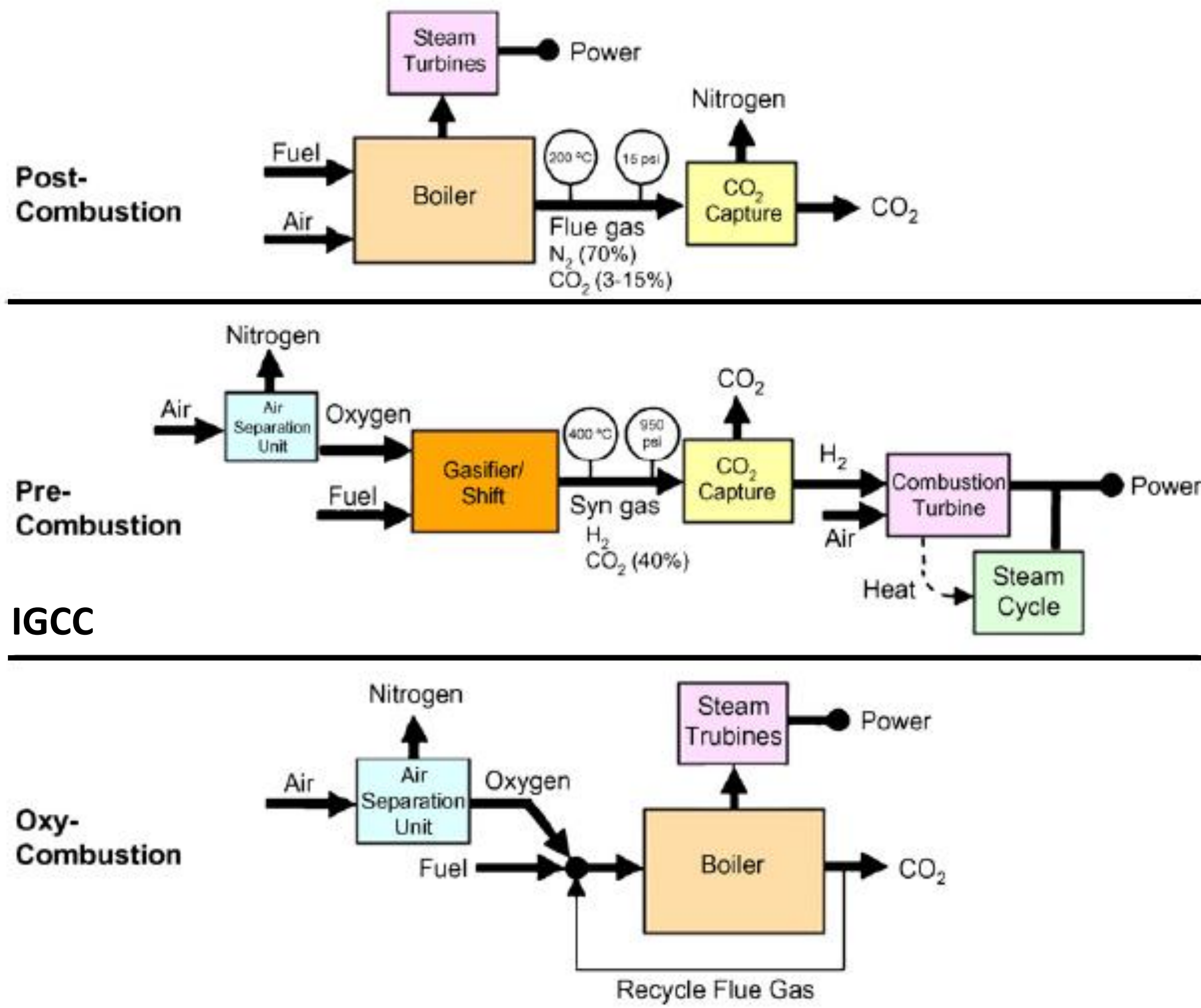
Carbon Capture and Sequestration



Two scenarios for reducing carbon dioxide emissions to keep atmospheric concentrations at 450-750 ppmv. Left: high-emission scenario, where nuclear plays an important role. Right low-emission scenario. In both cases, carbon capture and storage (CCS) – the orange wedge - plays a critical role. (IPCC report, 2007)

- **Continued use of fossil fuel while capping the atmospheric concentration of carbon dioxide to about double the pre-industrial level requires the sequestration of ~10 GT of CO_2 per year.**
- **Current technologies for the post-combustion capture of CO_2 are too expensive.**
- **"Underground" as a long-term storage container**
  - **Advantages: Enormous volume; distance from subsurface environment; pre-made container**
  - **Disadvantages: Designed by nature, only approximately fits the design criteria for containment; complex materials and processes; difficult to see and monitor; uncertainty about long-term performance**

Today's Carbon Capture Options



INTERNATIONAL JOURNAL OF GREENHOUSE GAS CONTROL 2 (2008) 9–20

Challenges

- Low CO_2 concentration
- High energy for regeneration

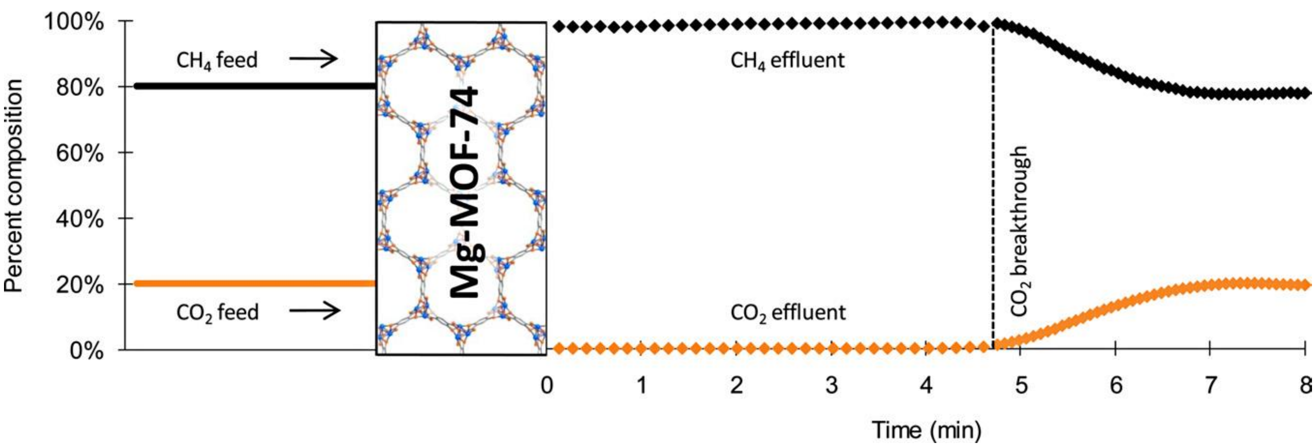
- Build new plants
- Oxygen production – expensive (chemical looping and ion transport membranes)

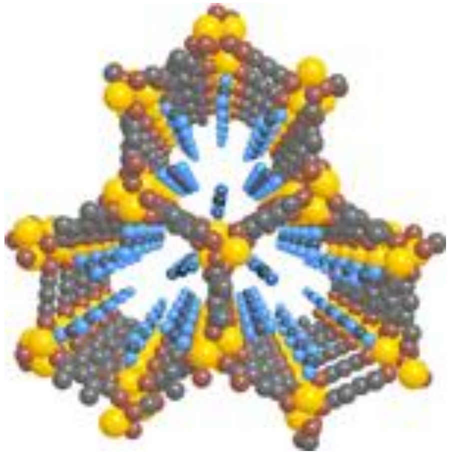
- Air Separation Units consume considerable energy
- Expense - corrosion resistant materials

New Materials May Aid in Capturing Carbon Dioxide Omar Yaghi, UCLA

Metal-organic frameworks (MOFs) act as "crystalline sponges" and show promise at reducing the energy penalty for CO_2 capture.

A new magnesium-based MOF is selective in capturing CO_2 in the presence of CH_4 and releases the stored CO_2 at temperatures much lower than current capture media.





Schematic structure of Mg-MOF-74

D. Britt, H. Furukawa, B. Wang, and O. M. Yaghi, PNAS 106, 20637 (2009); also featured in N.Y. Times on Dec. 8, 2009.

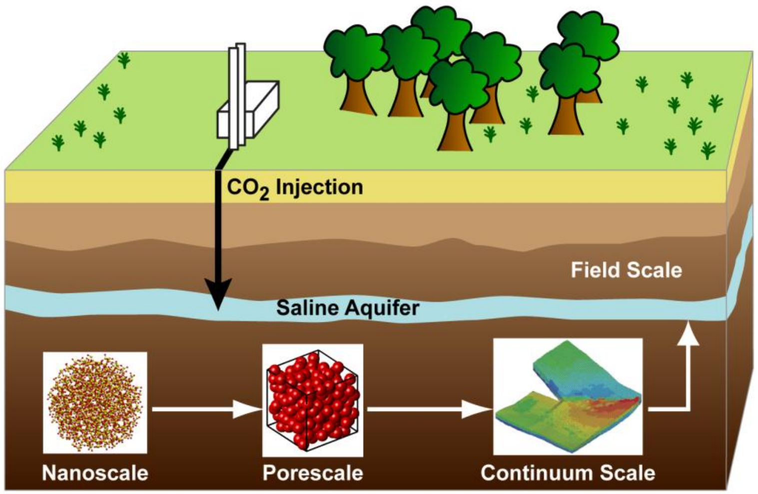
Geological CO_2 Sequestration

Geological Carbon Dioxide Sequestration is the deep well injection of supercritical CO_2 into porous rock formations for permanent disposal. This process initially displaces *in situ* aqueous fluid. Subsequently, the CO_2 buoyantly migrates slowly through the pores, breaking up into immobile bubbles, dissolving within the fluid, or reacting with minerals to form solid phases.

Prediction of CO_2 Sequestration effectiveness depends on understanding:

- **Reactive fluid flow properties of multiphase fluids under reservoir conditions in porous and fractured media**
- **Geochemical stability of mineral phases within deep formations**
- **Improved geophysical imaging of reservoir-scale properties to track changing reservoir dynamics over long periods of time**

EFRC: Center for Frontiers of Subsurface Energy Security
Gary. A. Pope (The University of Texas)



Summary statement: Our goal is scientific understanding of subsurface physical, chemical and biological processes from very small to very large scale so that we can predict the behavior of CO_2 and other byproducts of energy production that may need to be stored in the subsurface.

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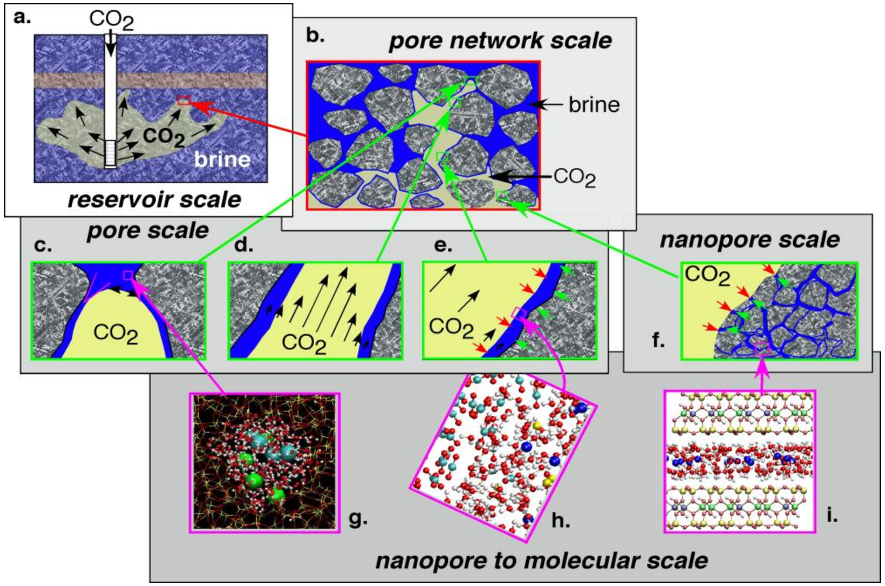
TEXAS

Sandia National Laboratories

EFRC: Nanoscale Controls on Geologic CO_2 -- Donald J. DePaolo (LBNL/ESD)



OBJECTIVES are to

(1) develop molecular, nano-scale, and pore network scale approaches for controlling flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; and

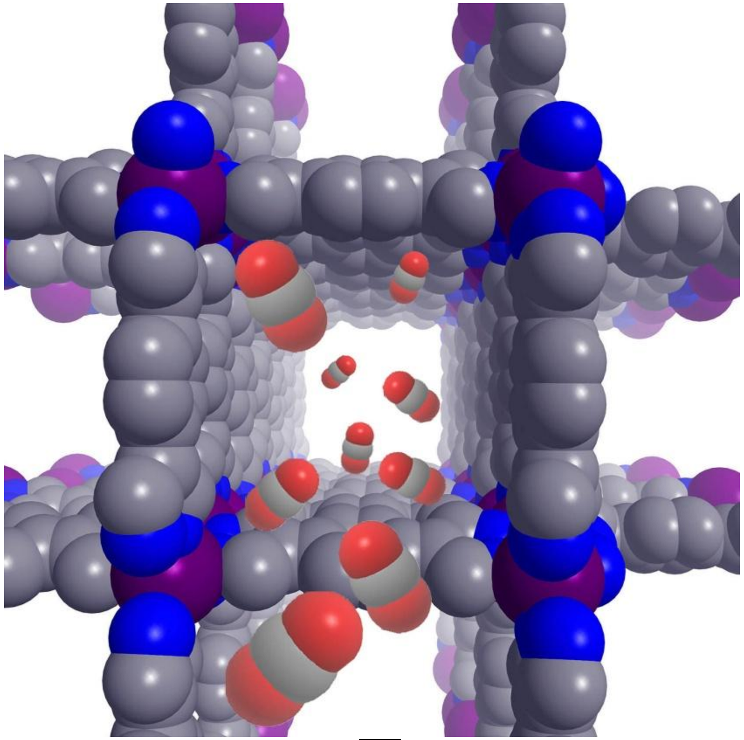
(2) achieve a new level of prediction of long-term performance

EFRC: Gas Separations for Clean Energy Technologies: (Smit, Berkeley)

Synthesis: Generate high surface area MOFs & self-assembled synthetic biomimetic polymer films

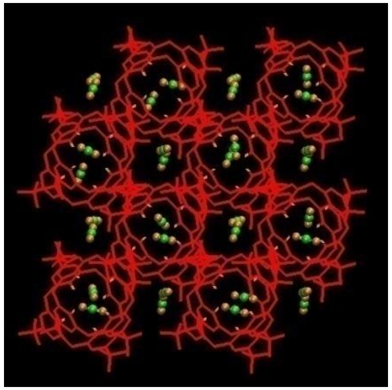
Characterization: Atomic-level structural characterization - before and after exposure to gas, accurate means of assessing the selectivity, kinetics, and thermodynamics of gas adsorbate binding – use to test computational models

Computational Separations: Strong computational component - understand chemical interactions at a molecular level, guide synthetic efforts



Goal: New strategies and materials for *energy efficient* selective *capture* or *separation* of CO_2 from gas mixtures based on molecule-specific chemical interactions

Examples of BES-Supported Projects in Theoretical and Computational Modeling



PNNL: Dang et al

One interpretation: Computer simulations show that at ambient temperatures, CO_2 molecules require ~ 4 times more energy than average to desorb. *Novel Strategies for selective heating may be necessary.*

Computational studies of load dependent guest dynamics and free energies of inclusion for CO_2 in low density p-*tert*-butylcalix[4]arene at loadings up to 2:1.

John L. Daschbach, Xiuquan Sun, Tsun-Mei Chang, Praveen. K. Thallapally, B. Peter McGrail, and Liem X. Dang. *J. Phys. Chem. A, Vol. 113, No. 14, 2009*

Theoretical and Computational Chemistry (Start FY09)**:** Modeling CO_2 capture and separation in zeolitic imidazolate frameworks (Wisconsin, Schmidt)

- Molecular Level Mechanism of CO_2 adsorption?
- Specificity of CO_2 over N_2 ?
- Mechanism for CO_2/N_2 Selectivity in ZIFs ?
- Thermal and Solvent Stability?