A Carbon Management Research Strategy

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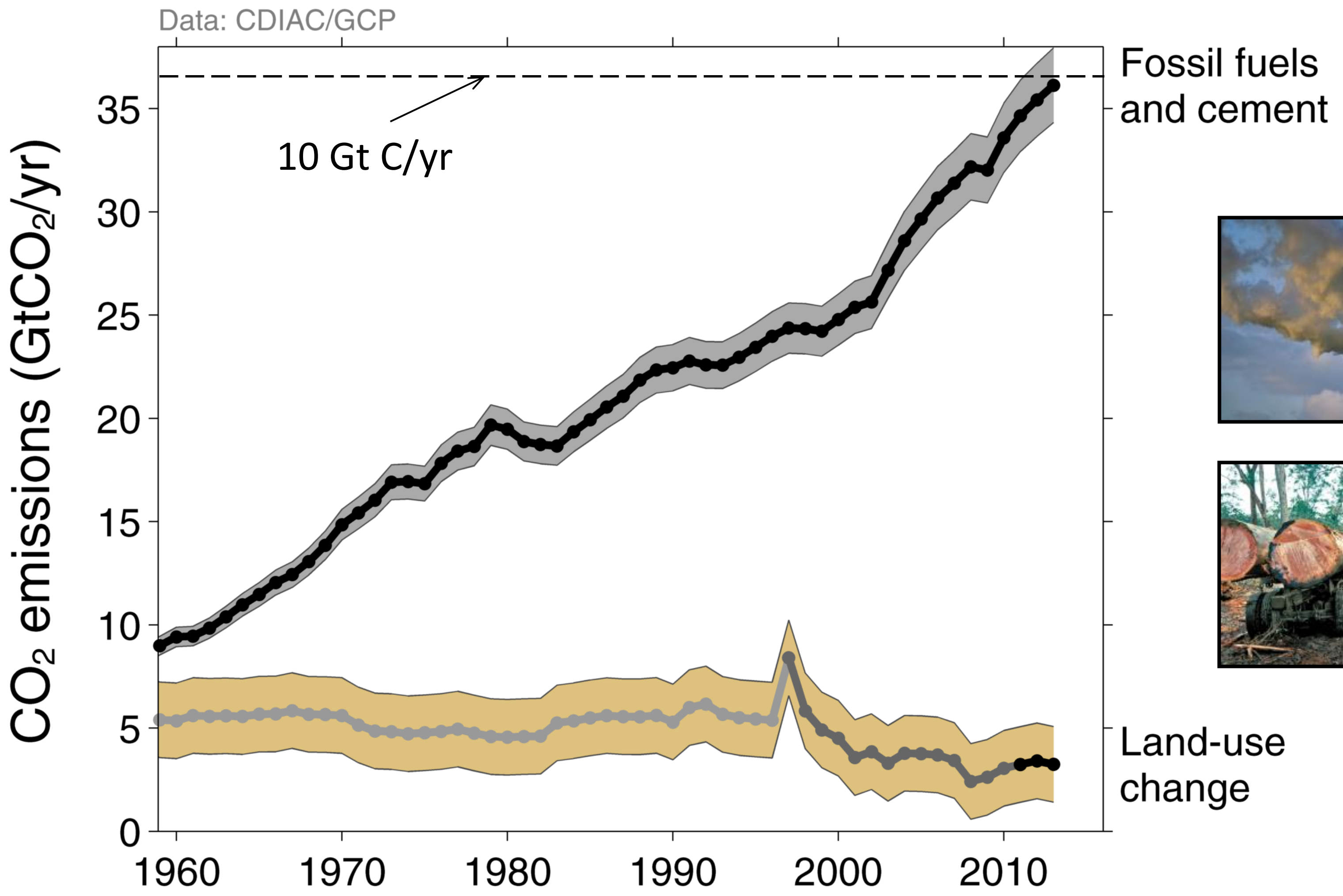
Center for Nanoscale Control of Geologic CO_2

NCGC

Outline

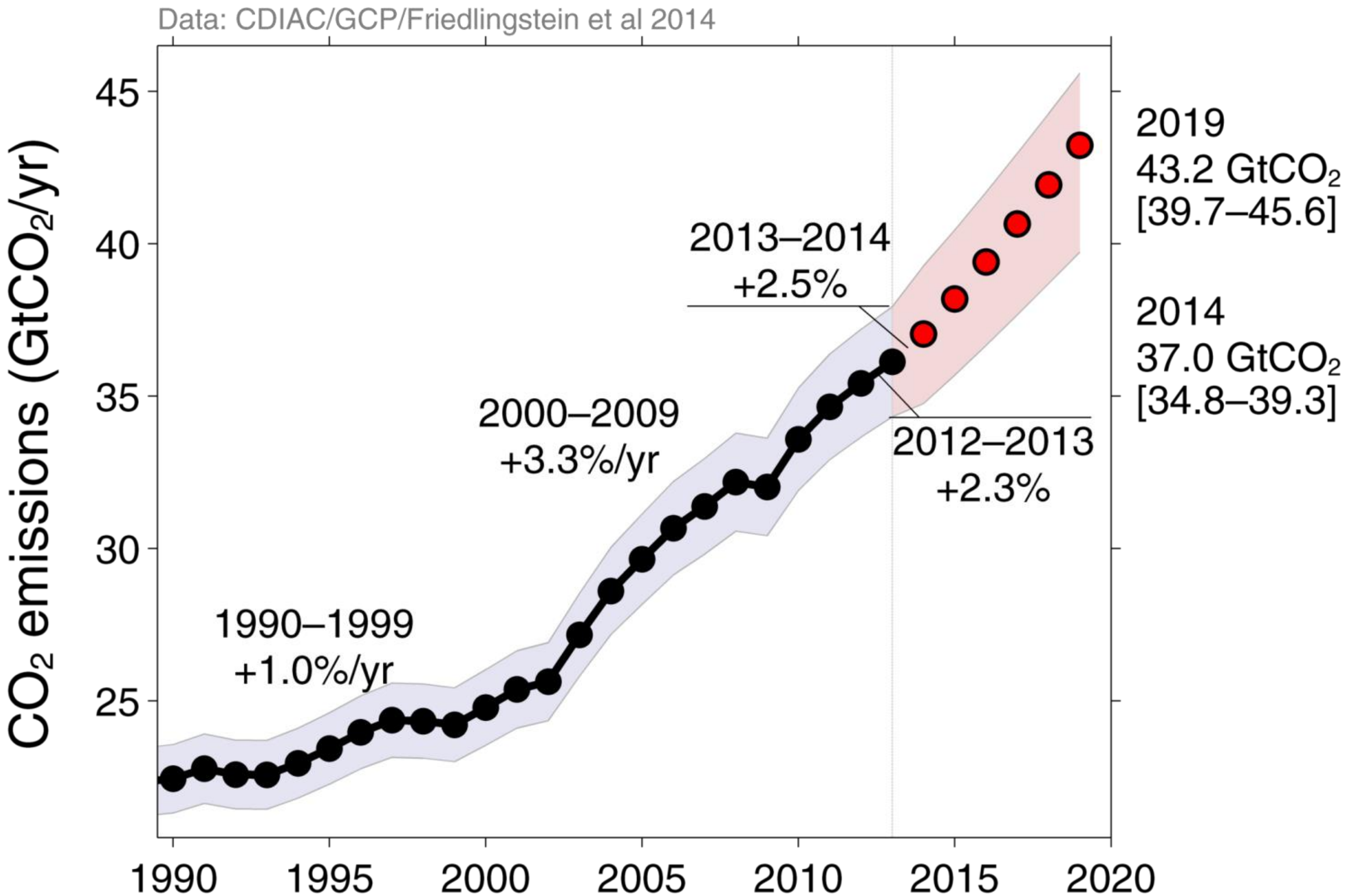
- Present carbon emissions and outlook. Humans in a pre-Human environment.
- The geologic view; what do we need to accomplish and when?
- Carbon intensity of energy production – ramping it down decade by decade
- CCS, Biofuels, and Artificial Photosynthesis.
- What about carbon Usage?
- Emphasis on aspects of the DOE R&D portfolio (it's not so bad!)

Total Global Emissions are not slowing down



Source: CDIAC; Houghton et al 2012; Giglio et al 2013; Le Quéré et al 2014; Global Carbon Budget 2014

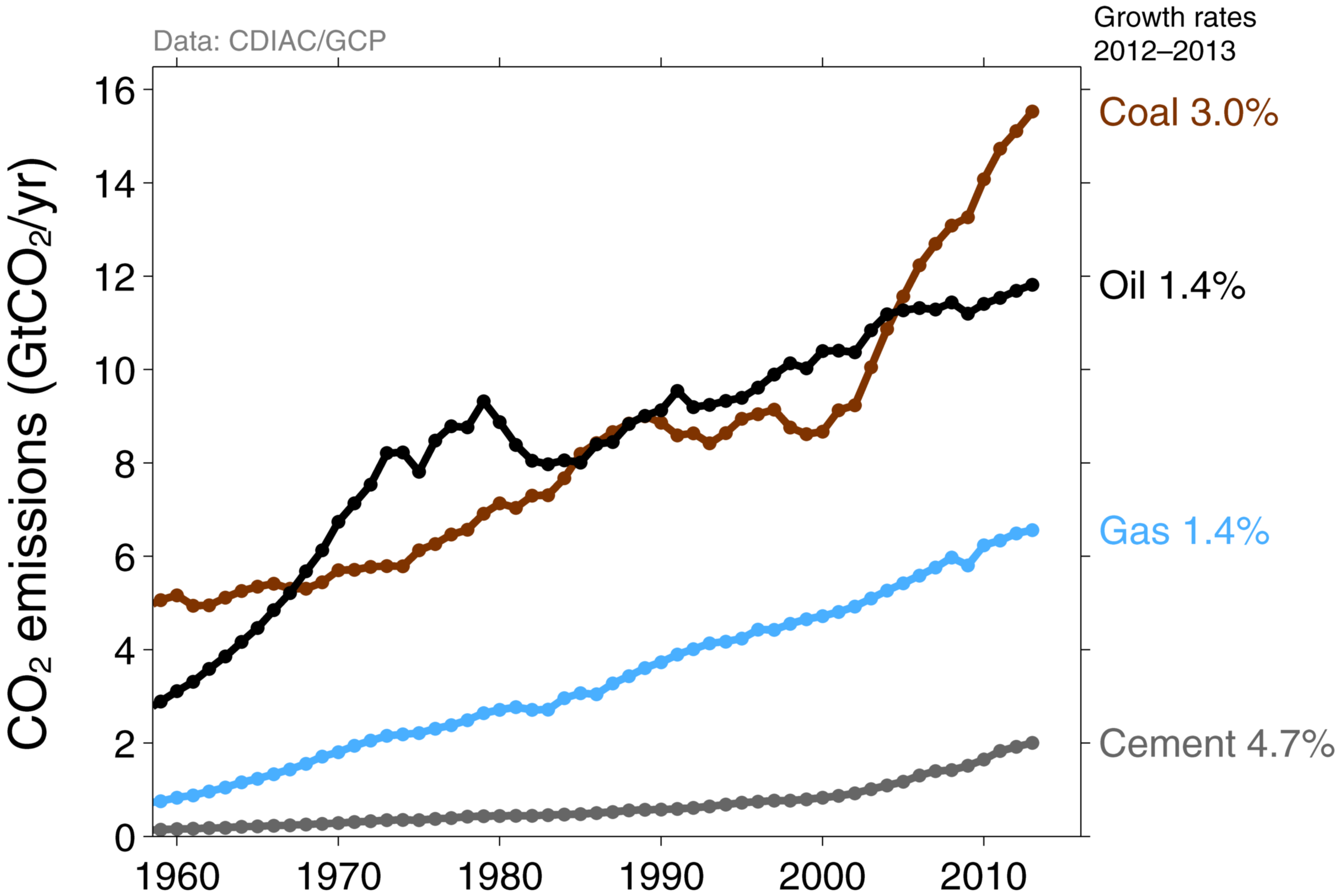
Near term outlook is not good



Economic growth based on IMF projections, fossil fuel intensity based on 10-year trend

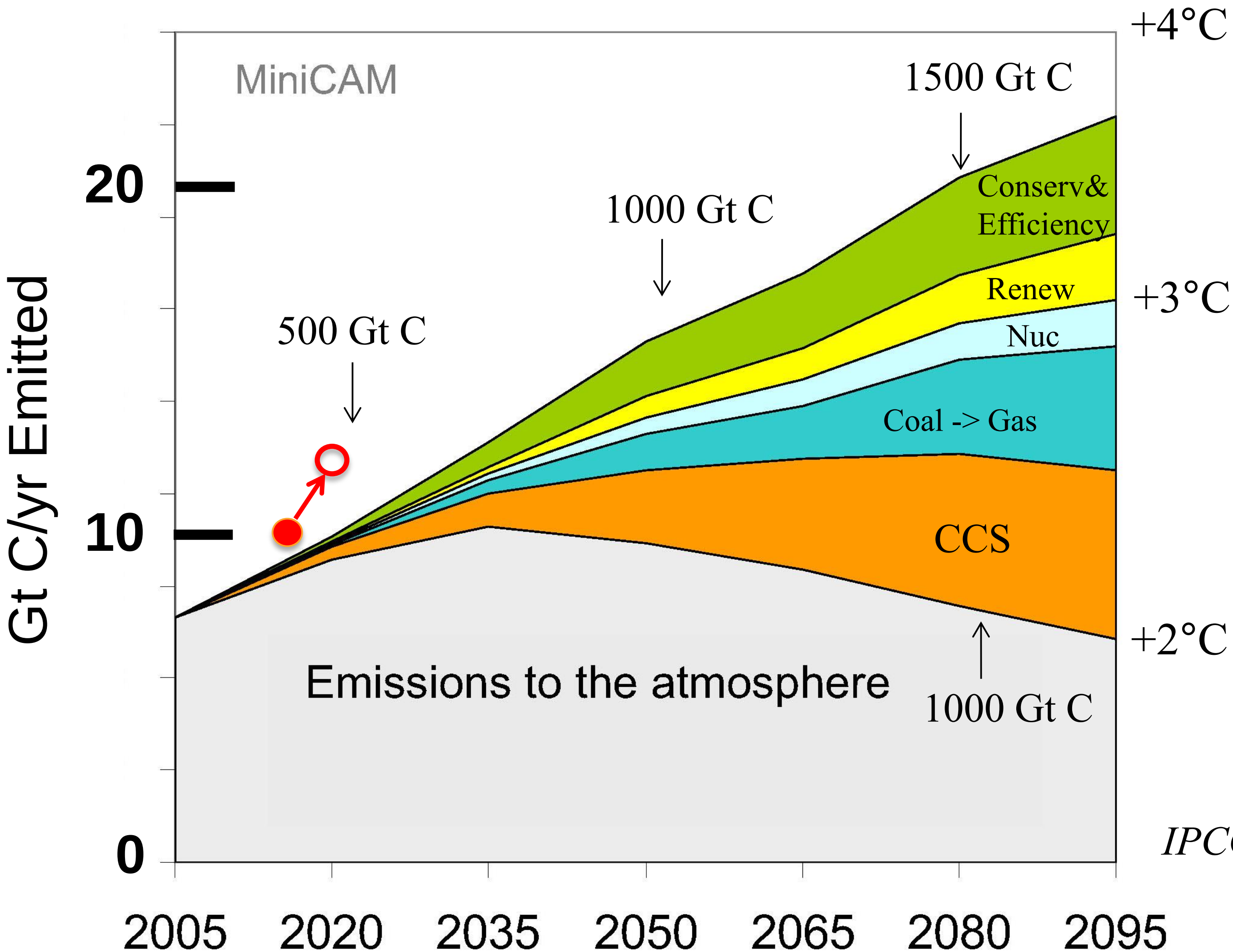
Source: CDIAC; Friedlingstein et al 2014

And coal is King again….



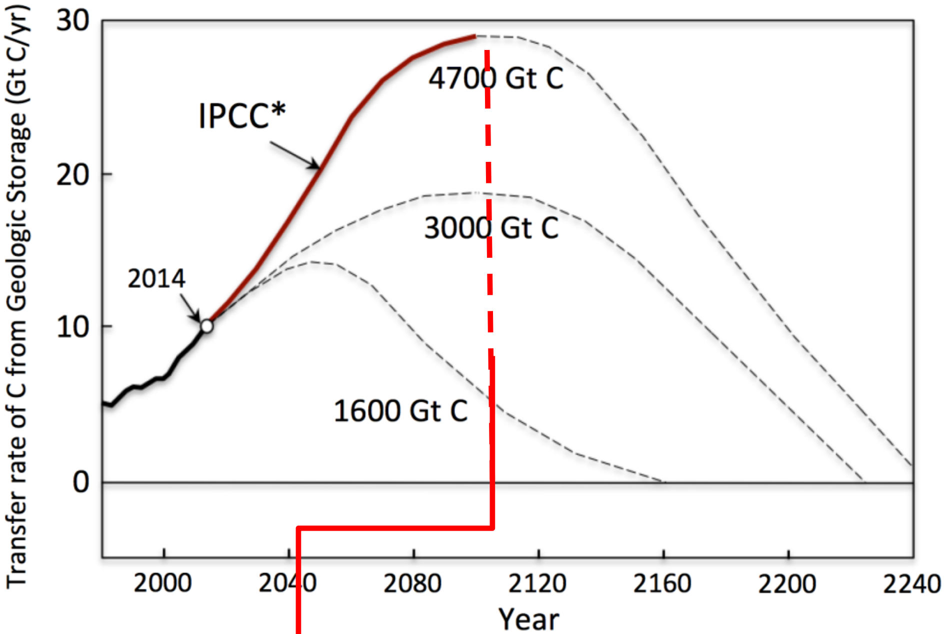
Source: CDIAC; Le Quéré et al 2014; Global Carbon Budget 2014

The most pessimistic IPCC 2005 projections of integrated carbon emissions now appear optimistic

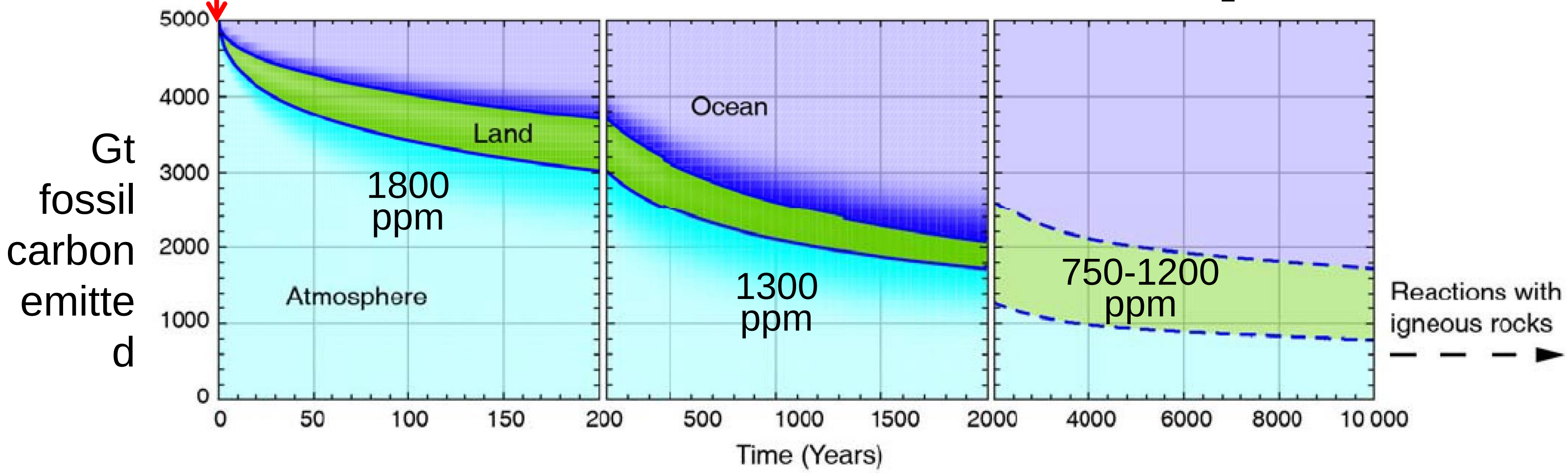


IPCC, 2005

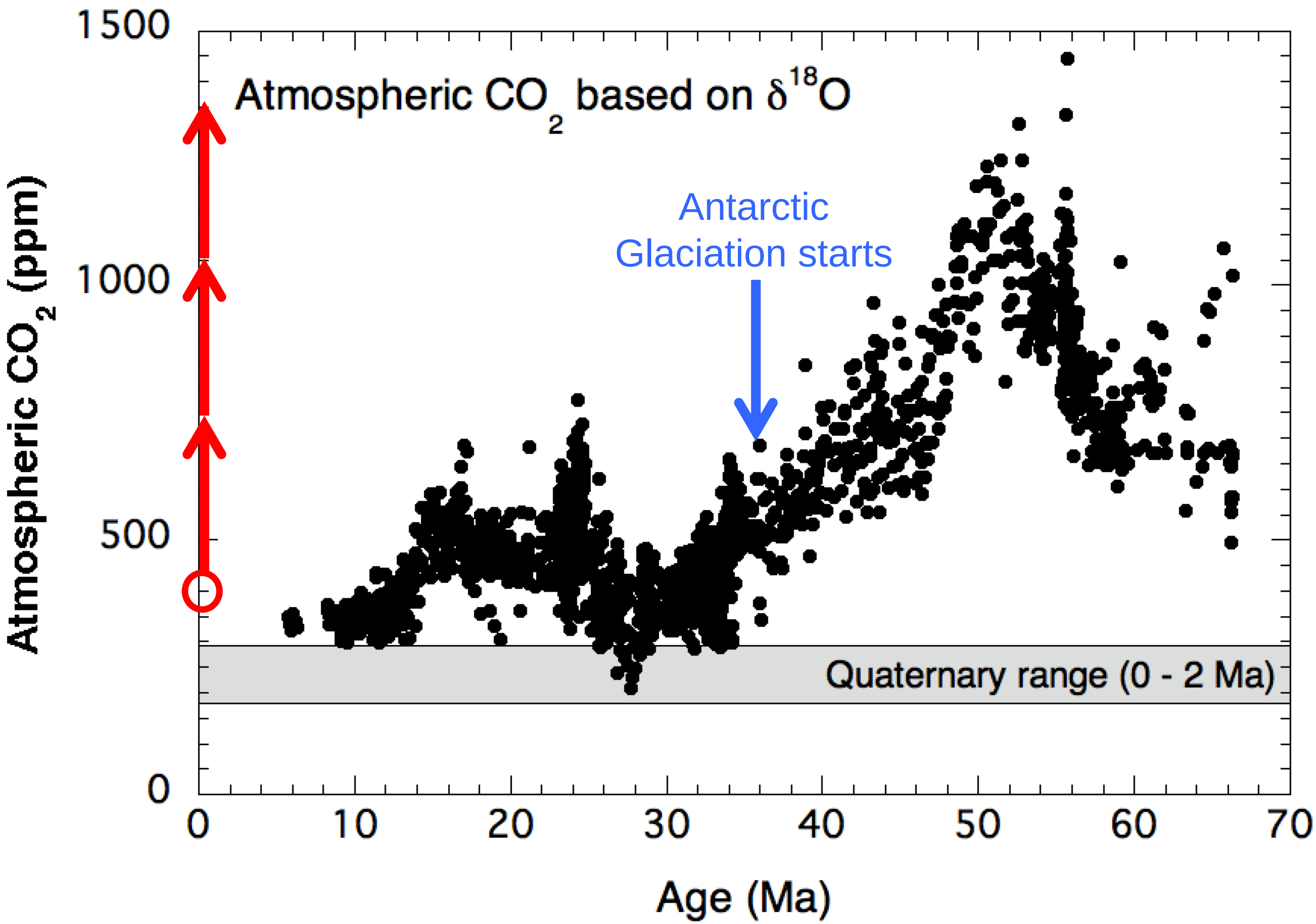
The next 100 years will make a huge difference



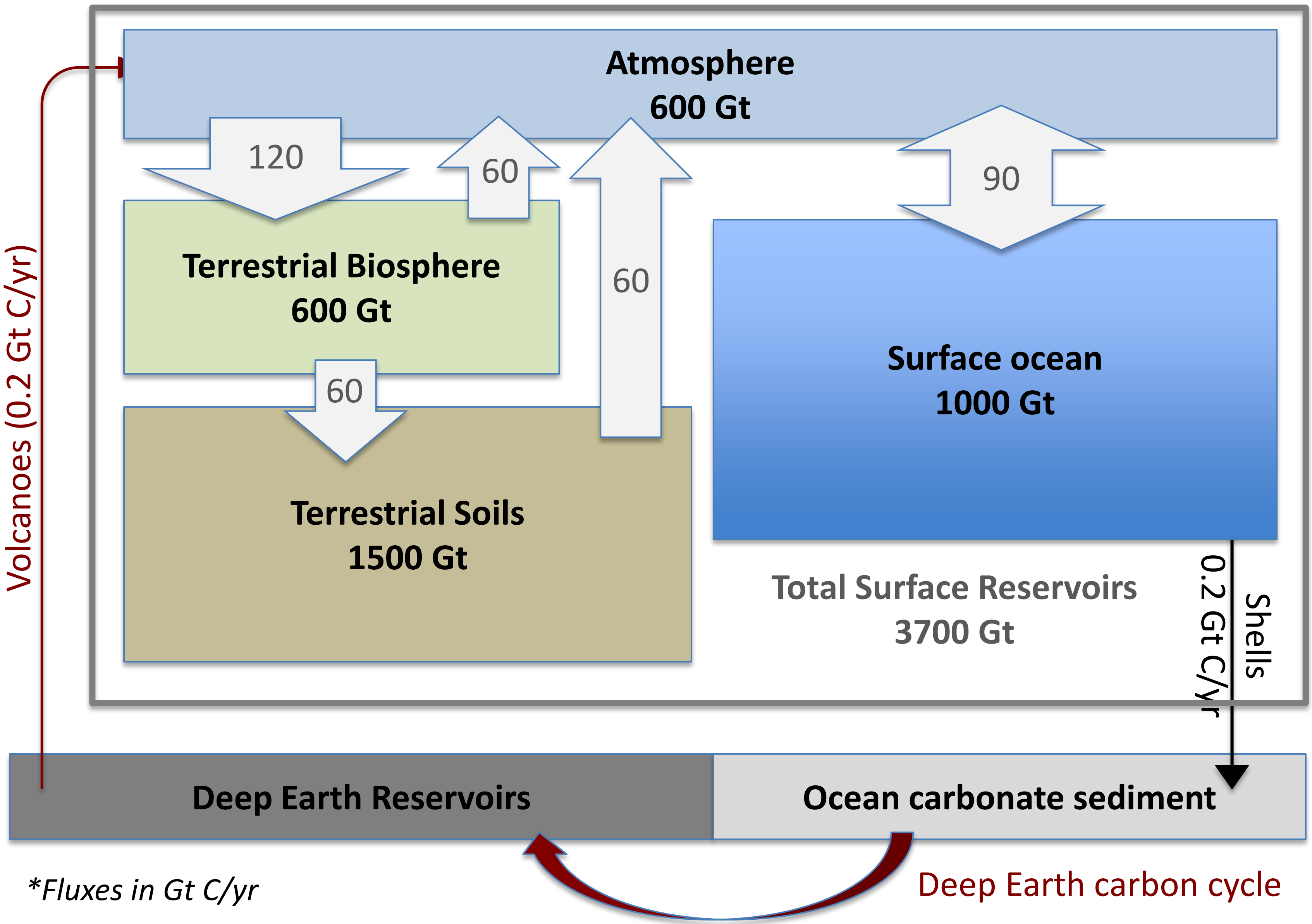
East Antarctic ice sheets unstable above 700 ppm CO_2



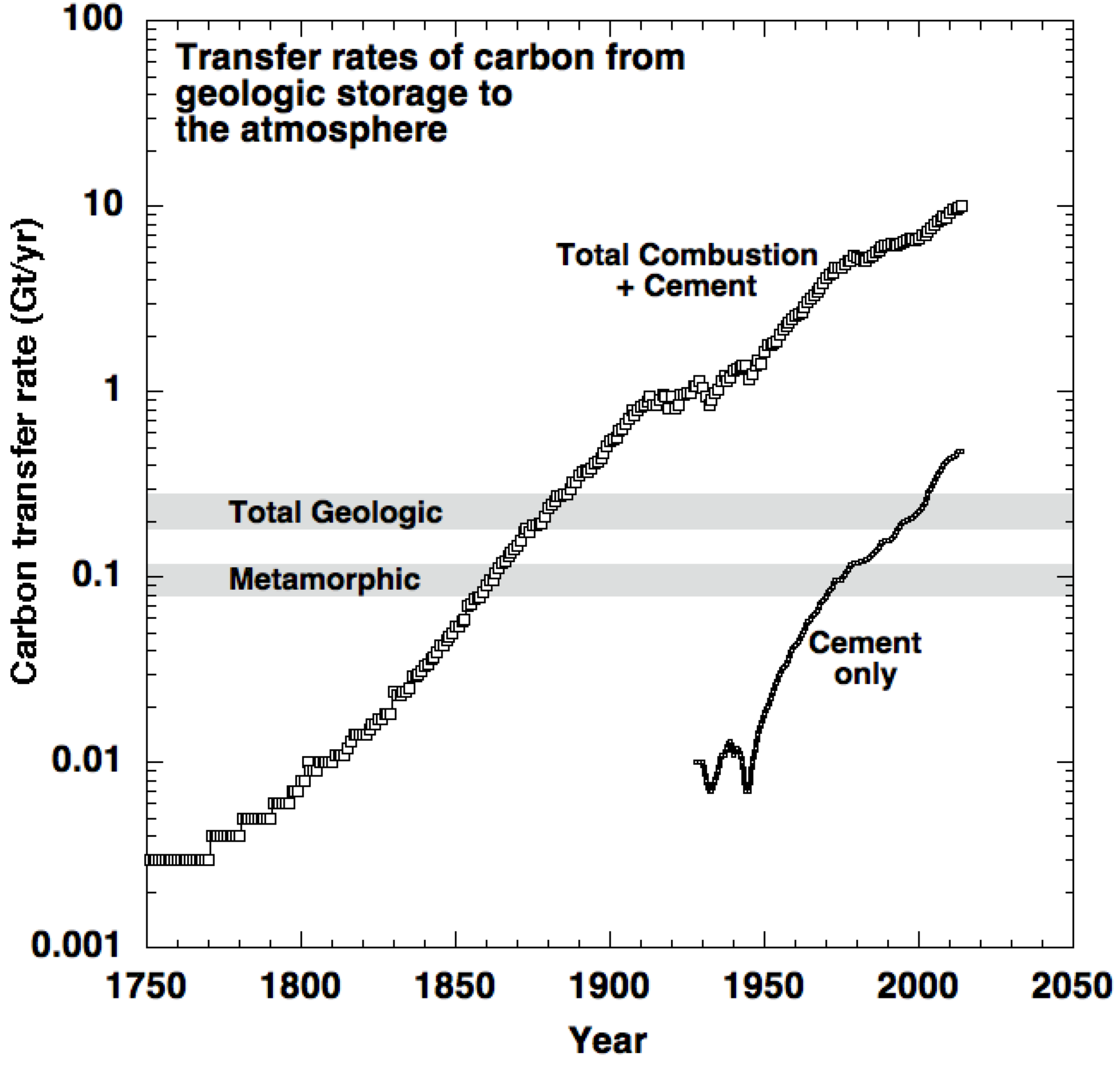
Turning the clock back….to pre-Human times



Box model version of global carbon cycle



*Fluxes in Gt C/yr

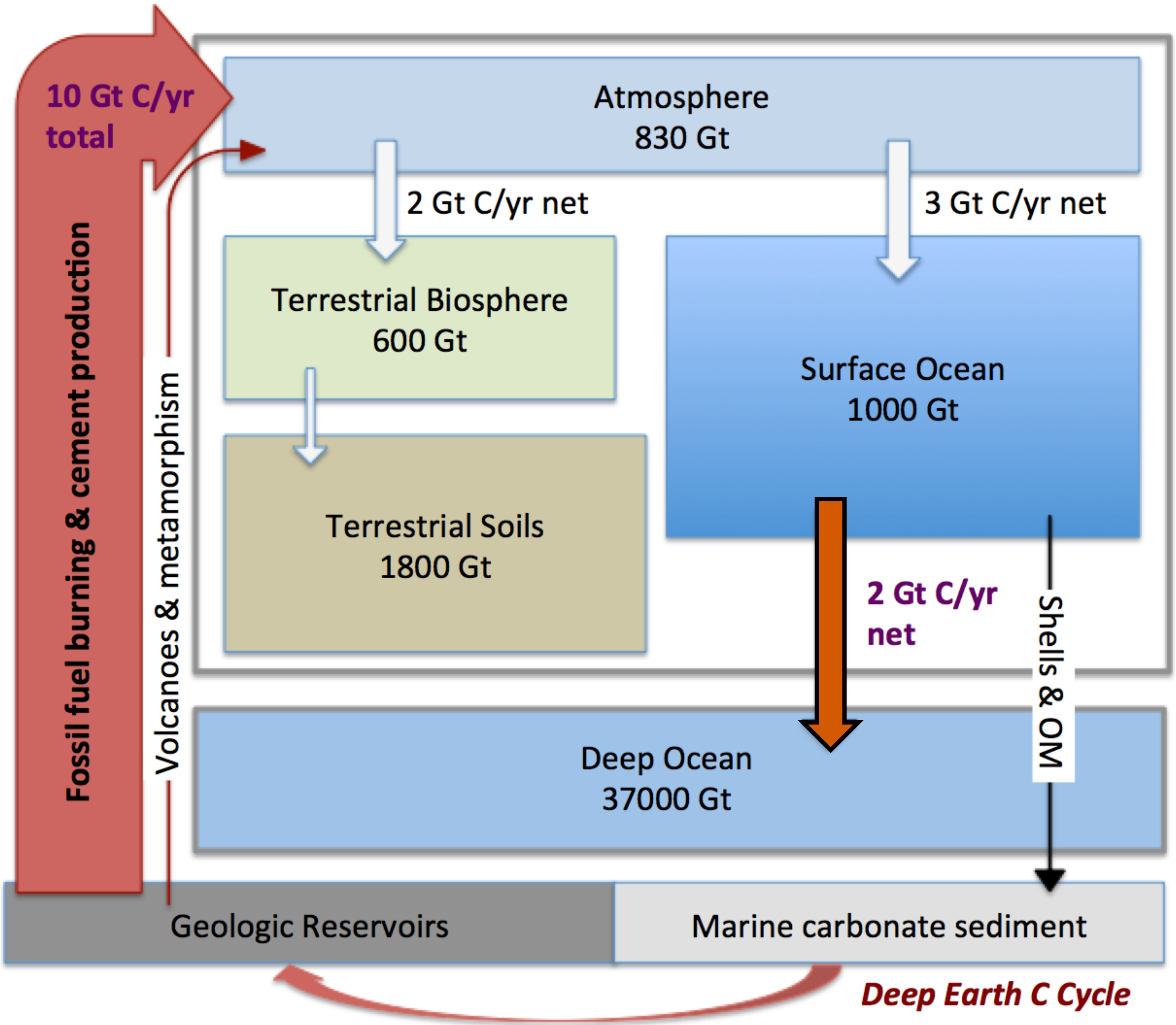


Anthropogenic C emissions from fossil fuels first exceeded the geologic rates in the late 19th century. Now they are ca. 50x higher.

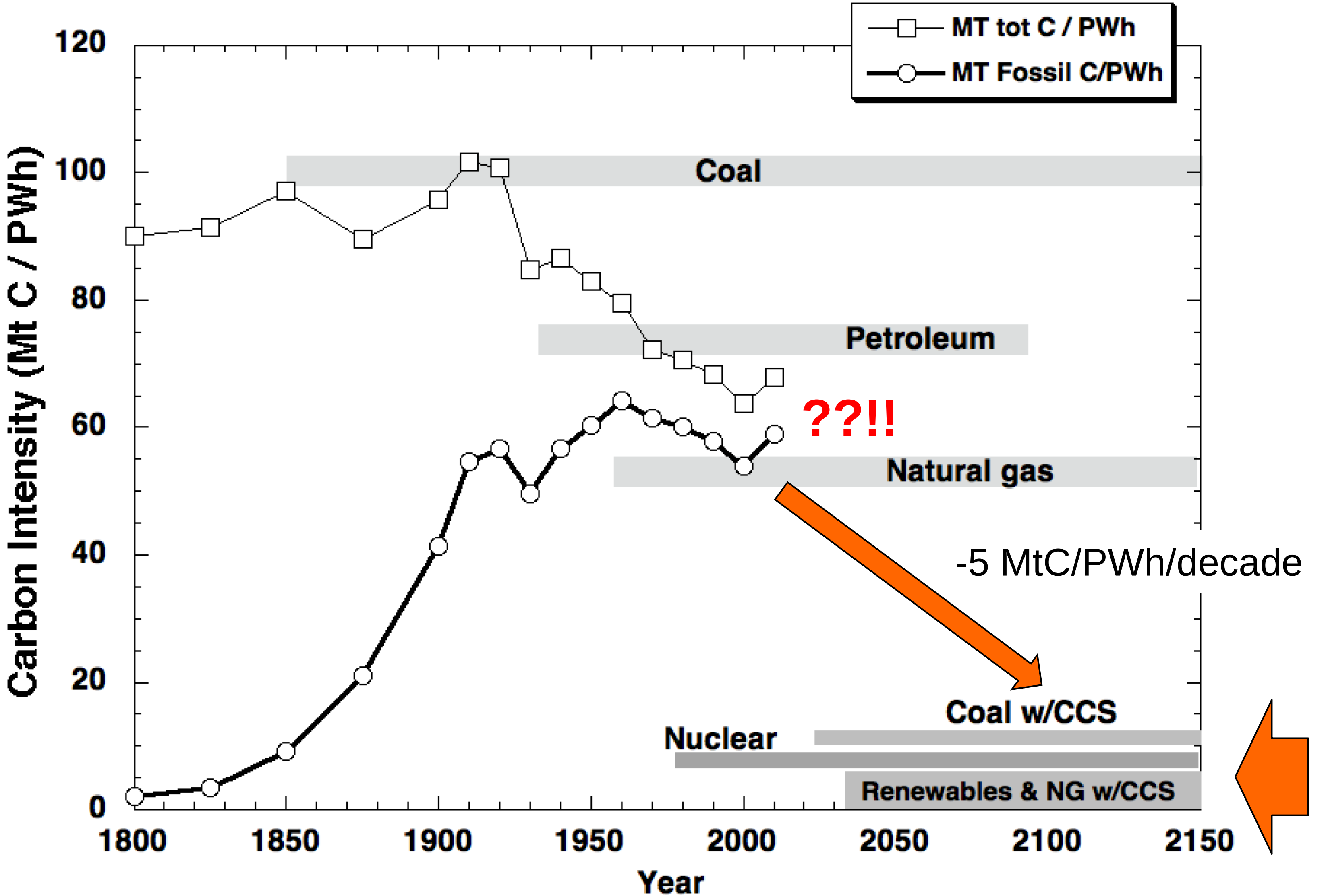
Data from ORNL database.

We are far beyond talking about natural or normal processes

Carbon cycle in 2015

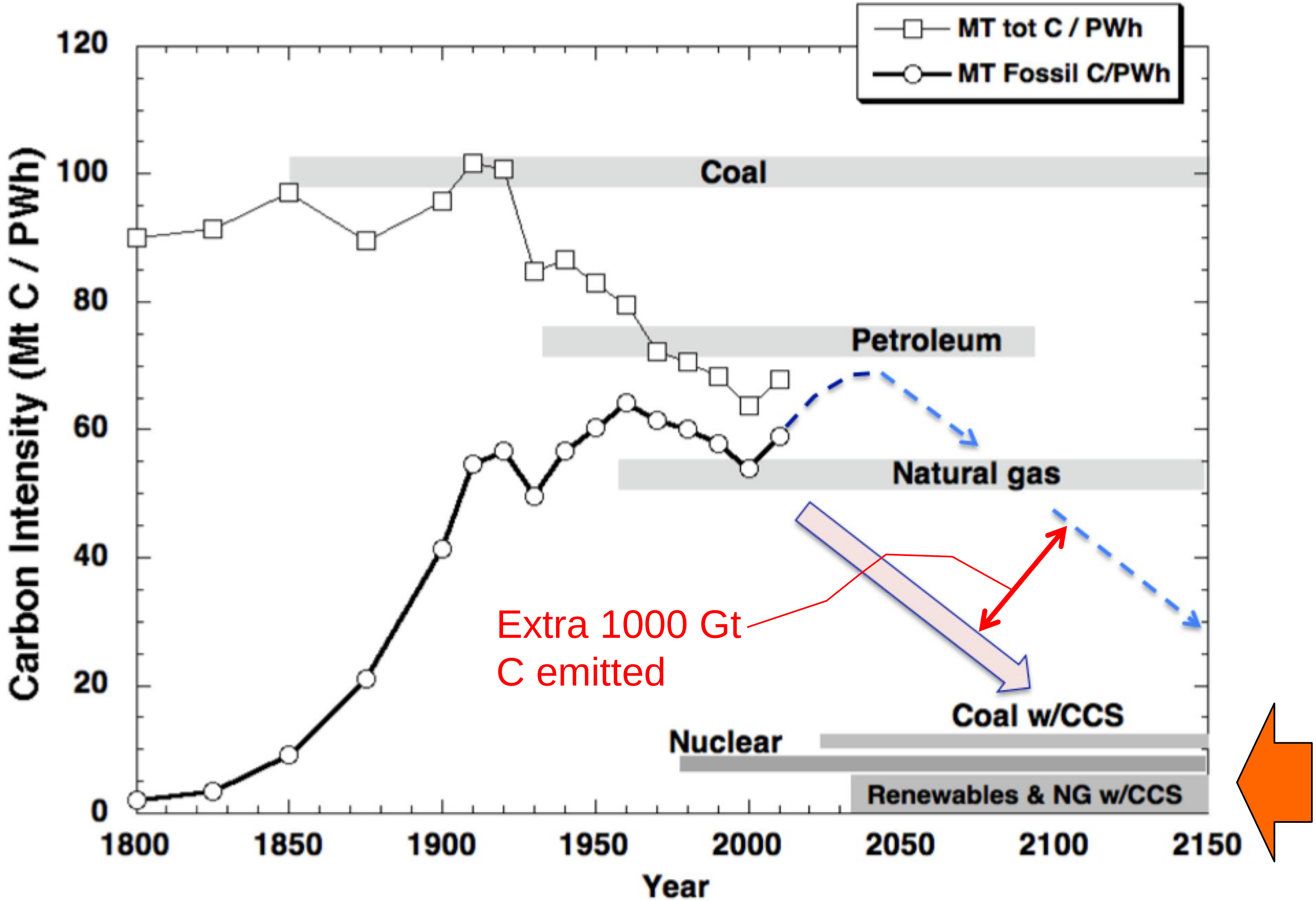


Carbon Intensity of Energy Production as Figure of Merit

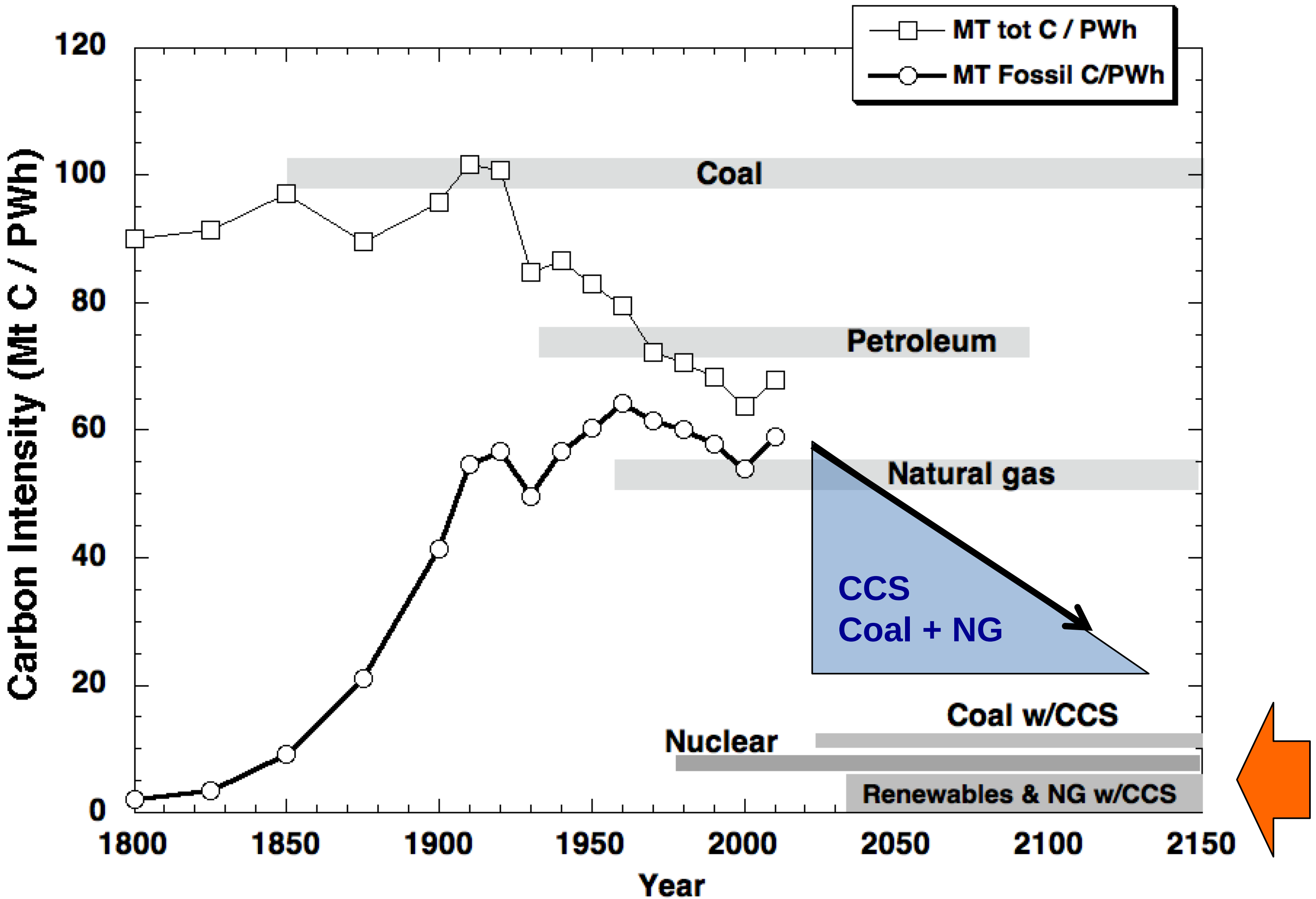


800 PWh at 5 MtC/PWh = 4 GtC/yr

Carbon Energy Intensity as Figure of Merit

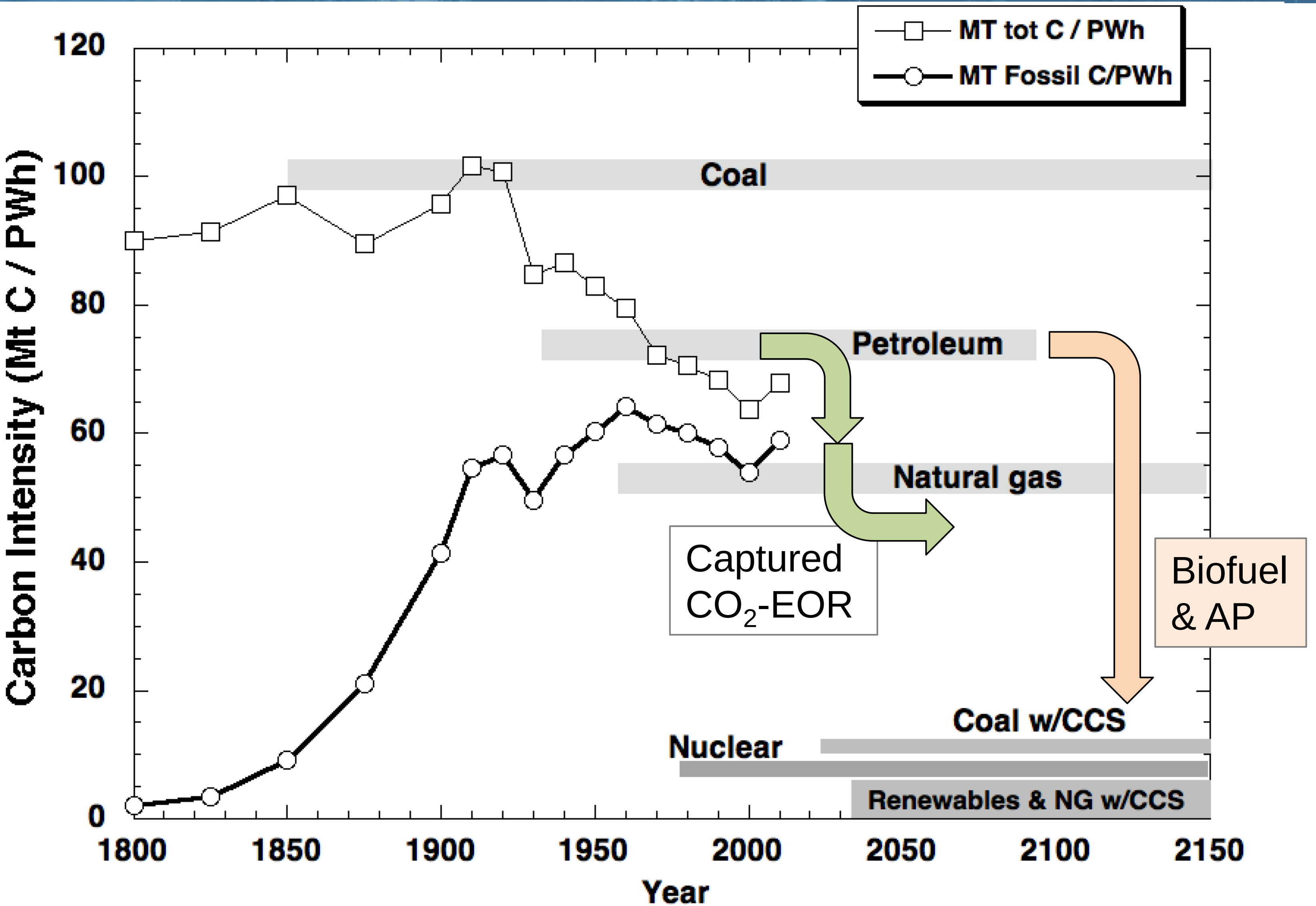


Getting there – CCS would allow for large scale continued energy production from Coal and NG

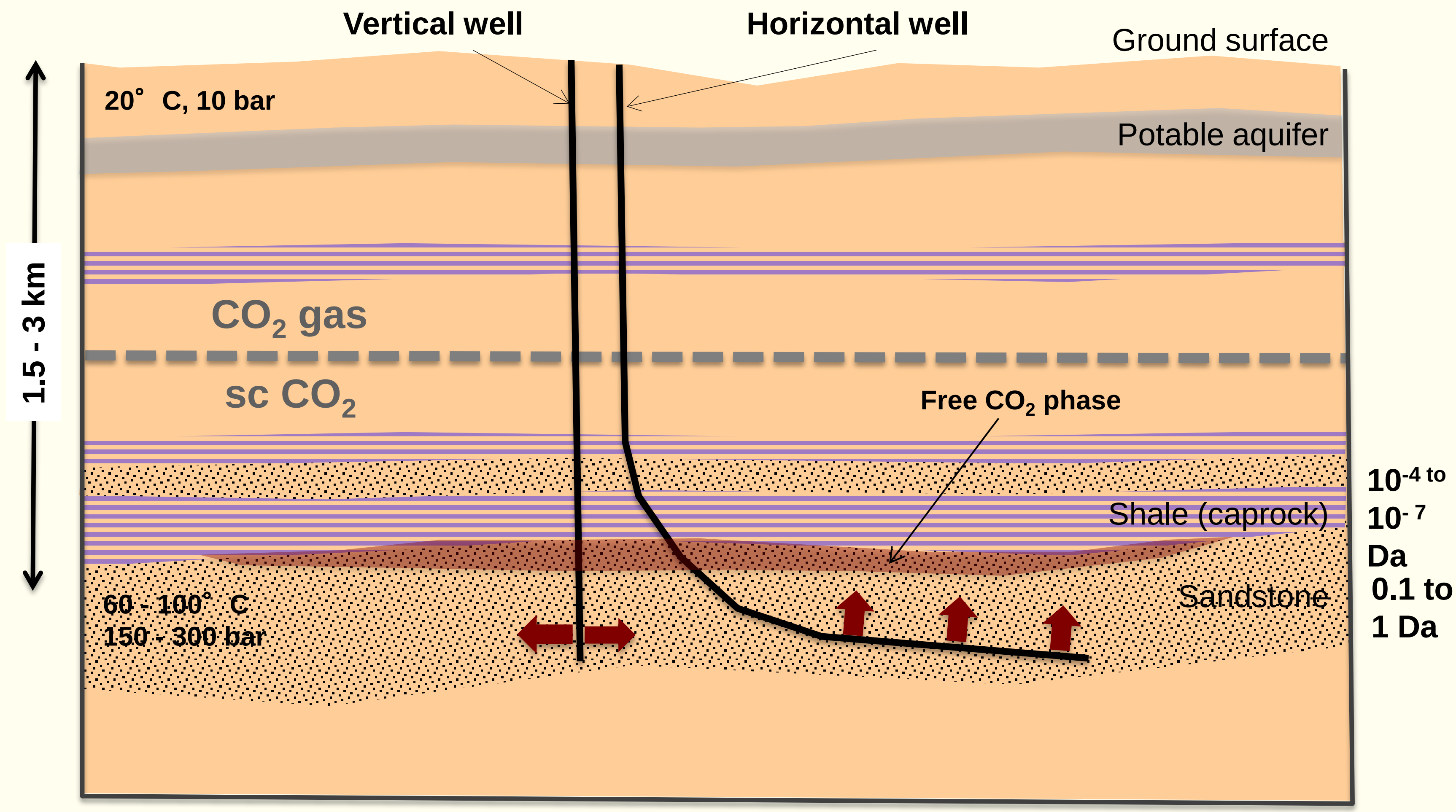


800 PWh at 5 MtC/PWh = 4 GtC/yr

Biofuels, AP, and even CO_2-EOR can help with liquid transportation fuels



Coal and Natural gas use means CCS is a requirement



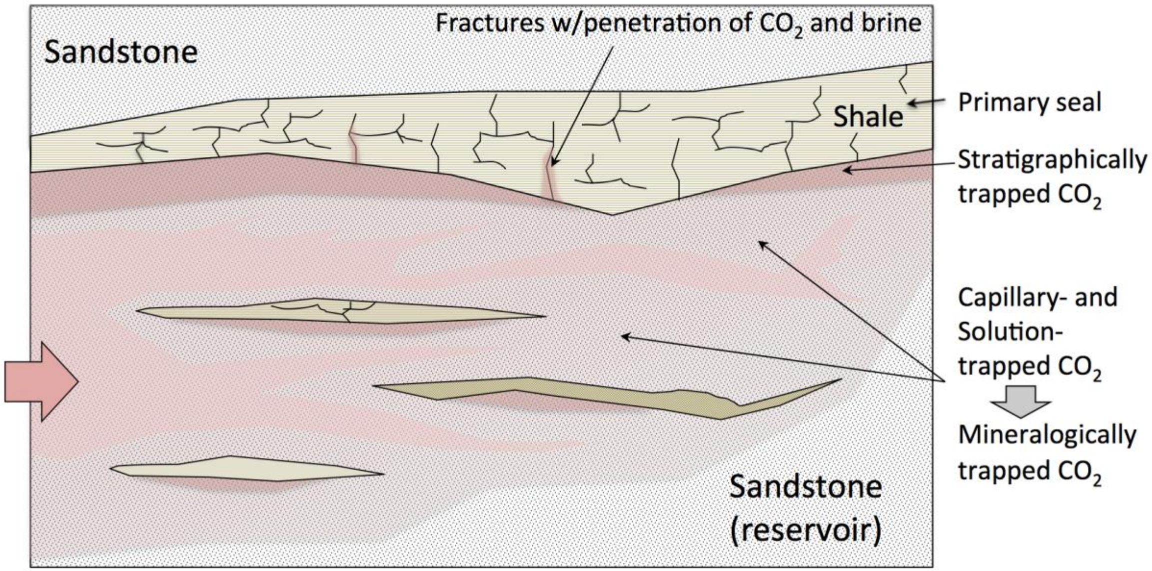
DOE Energy Frontier Research Centers

The U.S. DOE Office of Fossil Energy has recognized the critical role that Carbon Capture and Sequestration must play in reducing the CO_2 released to the atmosphere over the next 100 years.

There are demonstration projects underway in many parts of the U.S. and internationally, but the DOE *Office of Science* has also put new resources into *basic research* in the form of *EFRC's*.

1. ***Nanoscale Controls on Geologic CO_2 (NCGC; LBNL lead)***
2. ***Subsurface Energy Security (CFSES; Texas Austin lead)***
3. ***Geological Storage of CO2 (GSCO2; U. Illinois lead)***

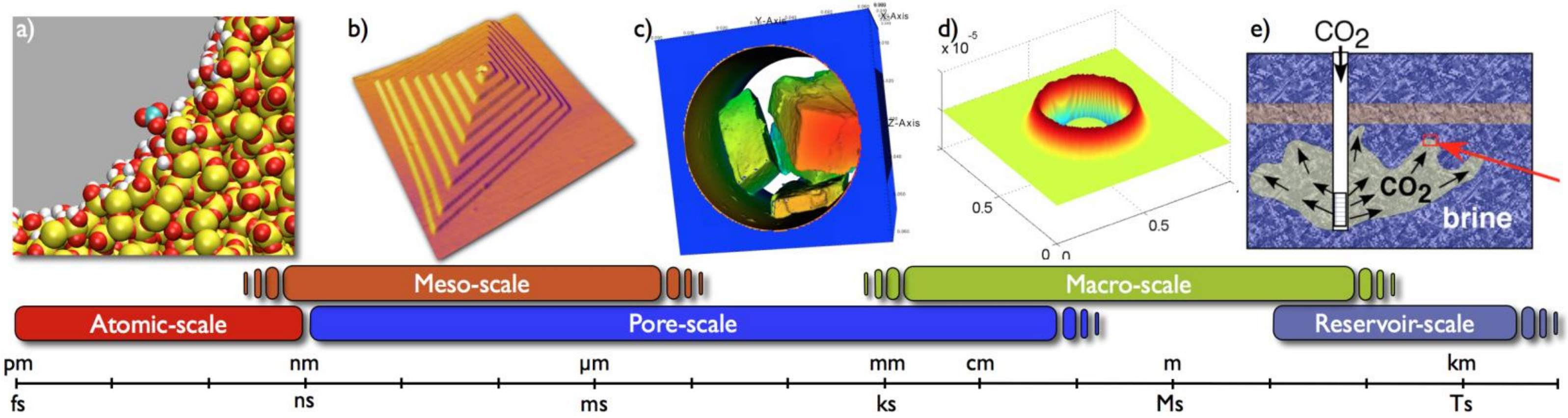
Some GCS basic research questions …..

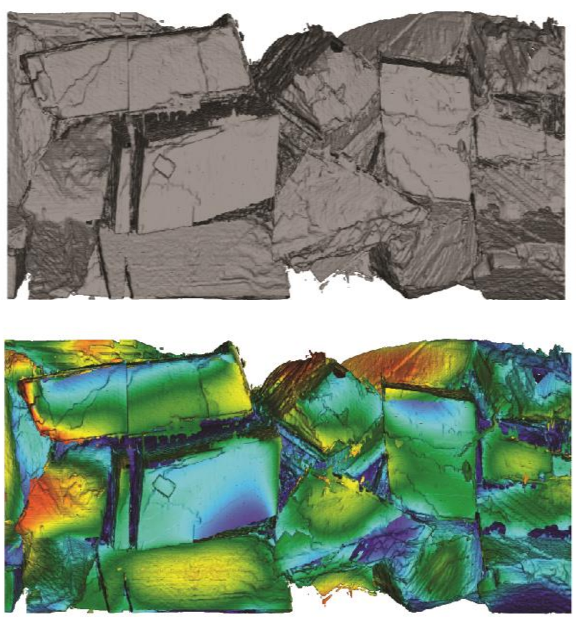


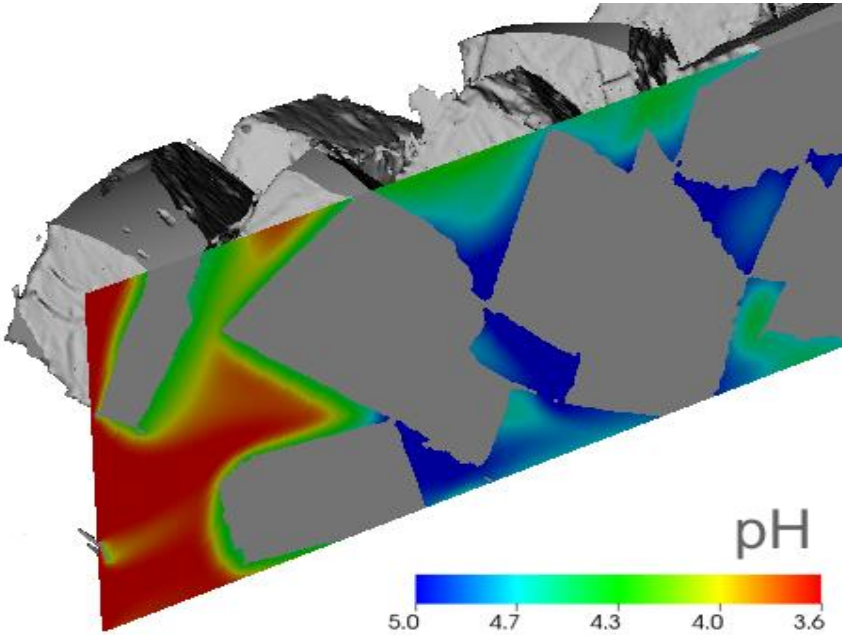
Questions:

1. How much CO_2 is likely to be accounted for by capillary trapping? What does it depend on?
2. Is capillary trapping permanent, or can it break down on longer timescales due to chemical processes?
3. Will geochemical reactions affect the capacity and security of shale seals if they are fractured or faulted and/or fractured during injection?
4. Can a significant fraction of the injected CO_2 be converted to carbonate on a 1000-year time scale?

Attempting to deal with scales….







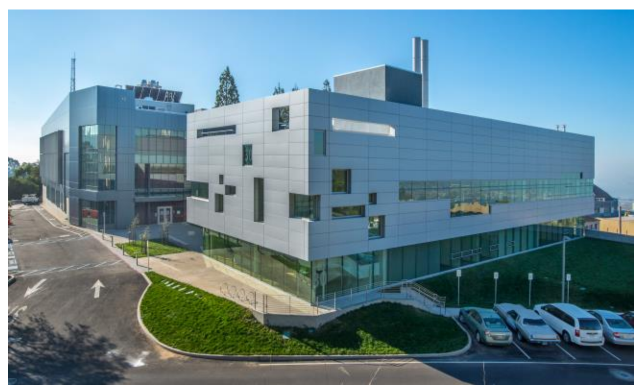
LBNL Major Research Facilities

Advanced Light Source

National Energy Research Scientific Computing Center

Joint Bio-Energy Institute

Molecular Foundry



Solar Energy Research Center

National Center for Electron Microscopy

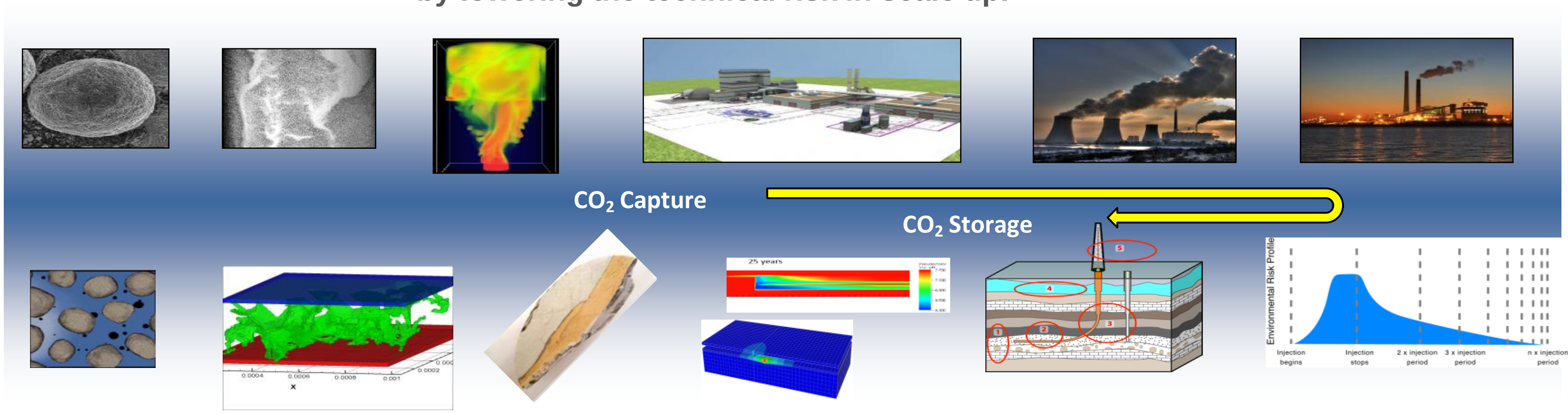
Tools for advancing CCS technology

Leveraging DOE's Science-Based Prediction Capability
to Build Confidence in Engineered–Natural Systems

Carbon Capture Simulation Initiative (CCSI)

To accelerate the path from concept (bench) to deployment (commercial power plant) by lowering the technical risk in scale up.

CCSI

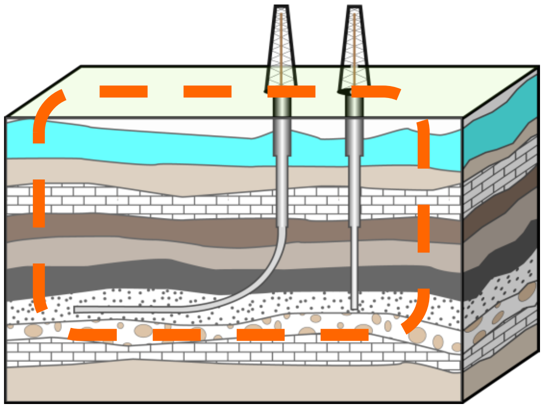


NRAP
National Risk Assessment Partnership

National Risk Assessment Partnership (NRAP)

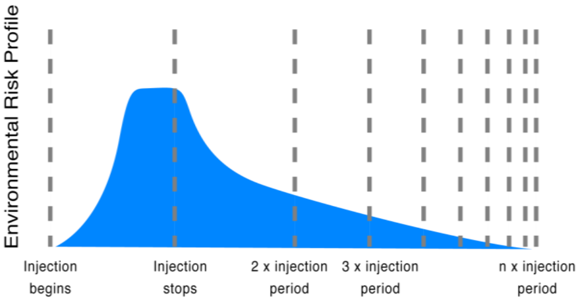
To accelerate the path to CCUS deployment through the use of science-based prediction to quantify storage-security relationships, thereby building confidence in key decisions.

NRAP: Science-based prediction to build confidence in storage security by quantifying system performance for multiple conditions.

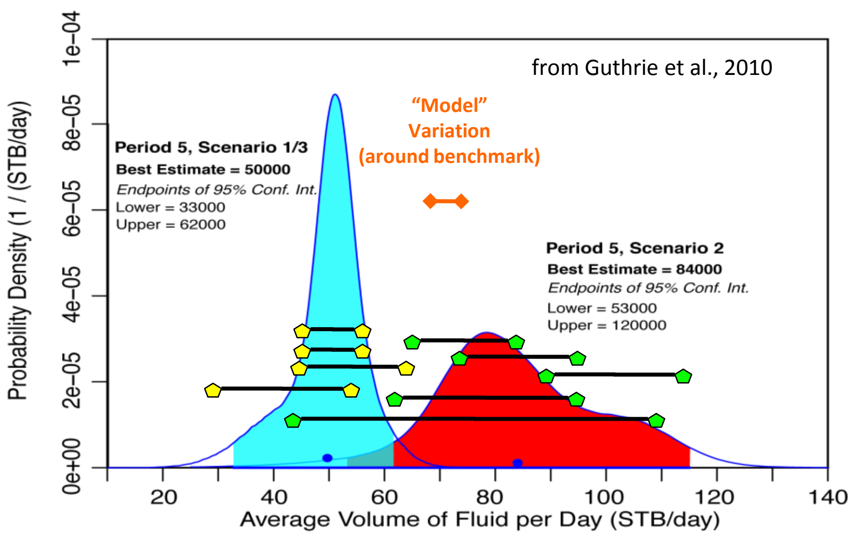


NRAP Goal—to predict storage-site behavior from reservoir to receptor and from injection through long-term storage…

…in order to quantify key storage-security relationships for various site characteristics.

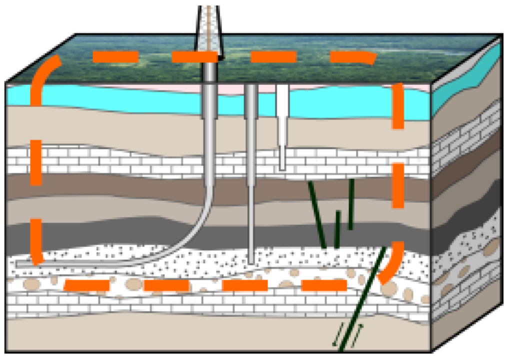


Confidence in uncertain predictions can be built through comprehensive, multi-organizational team assessments.



NRAP is building and applying computationally efficient tools to probe site behavior stochastically, thereby accounting for uncertainties and variability in storage-site characteristics.

Assessing risks in complex geosystems



NRAP Goal—to predict storage-site behavior from reservoir to receptor and from injection through long-term storage…

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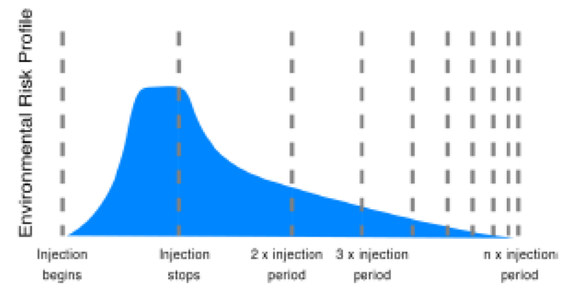


Challenge

- Large, complex system
- Uncertain geologic parameters
- Prediction of processes that cannot be directly tested or observed
- **Site-specific characteristics**

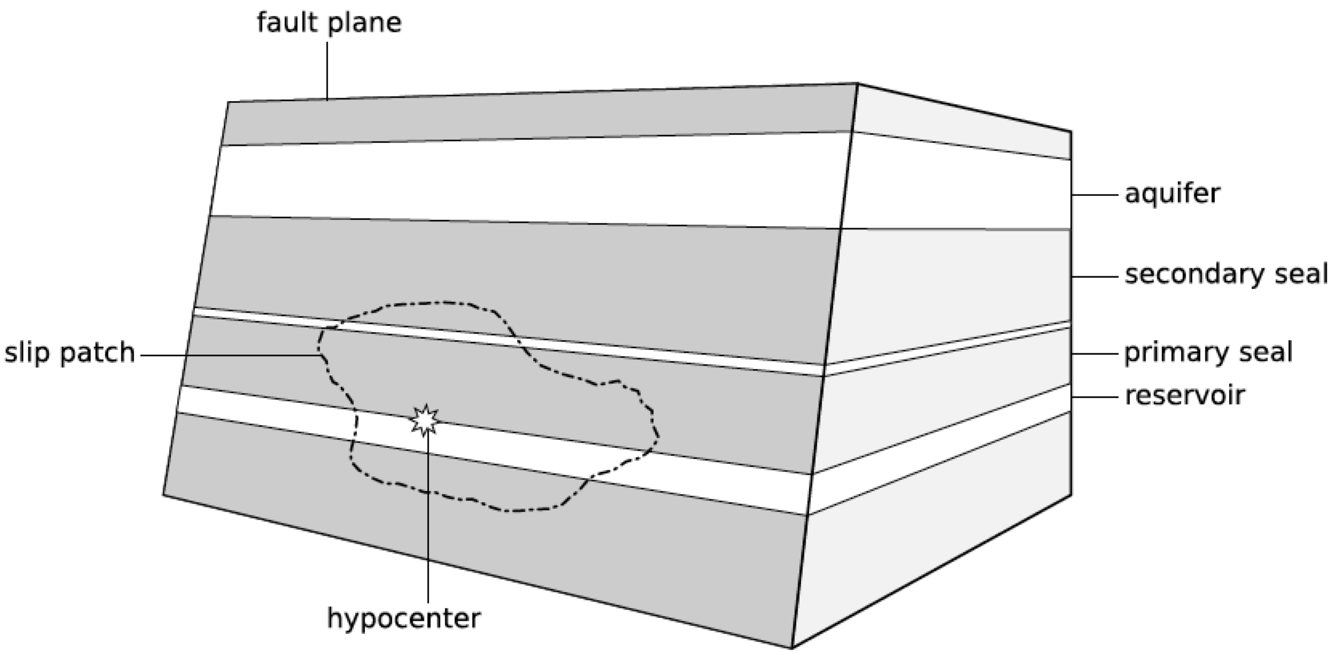
NRAP Approach

- Utilize integrated assessment models that break the system into smaller pieces
- Utilize reduced order models that run rapidly coupled with Monte Carlo methods
- Utilize high-fidelity, physics-based models to characterize critical behavior
- **Build in flexibility for utilizing site-specific information, including data generated by reservoir simulators based on site models**

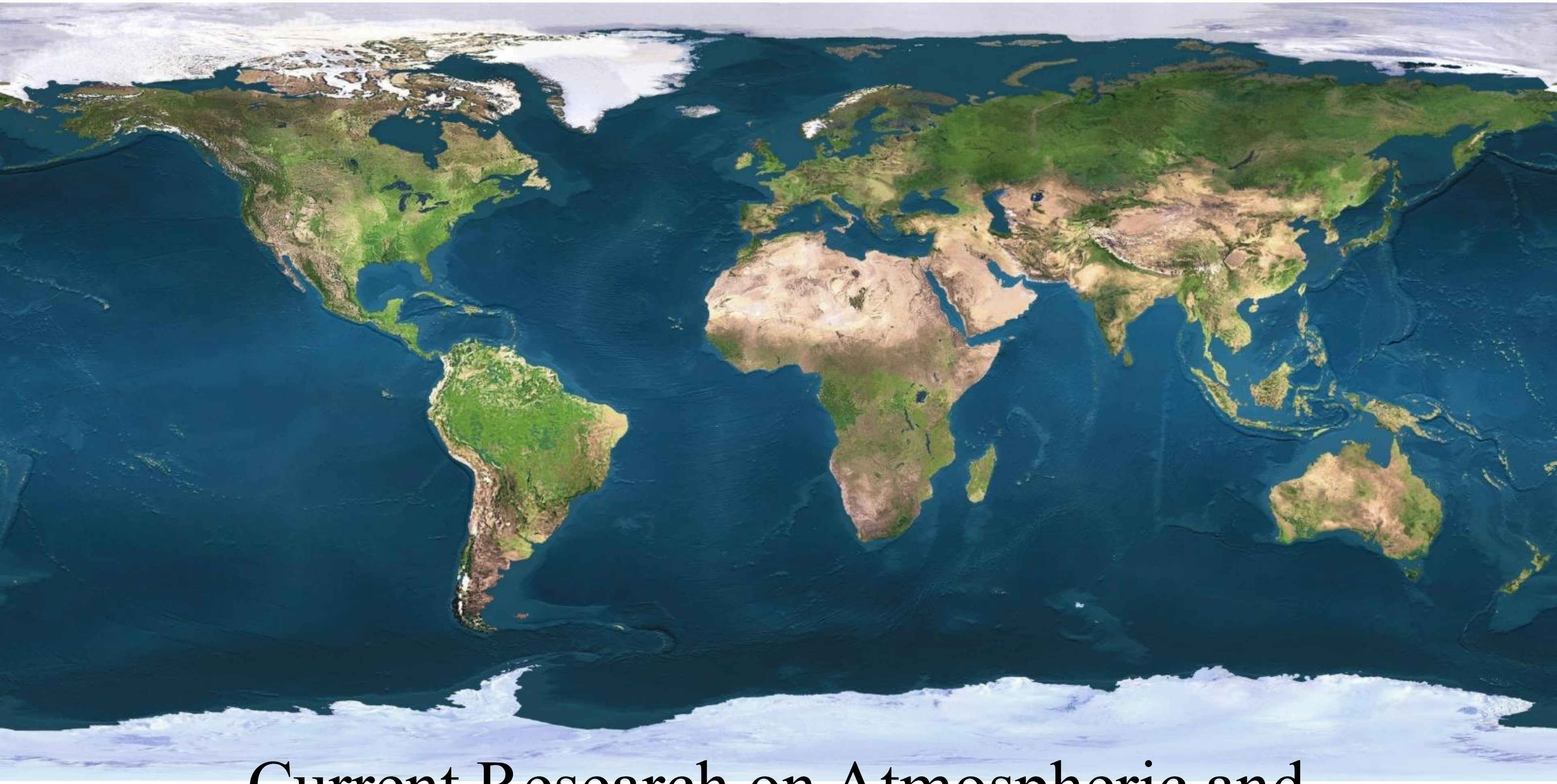
Induced seismicity working group

① Identify site characteristics and operations that lead to low-risk—i.e. minimal hazard, minimal damage.

② Develop techniques to quickly identify and manage seismicity problems if they should appear

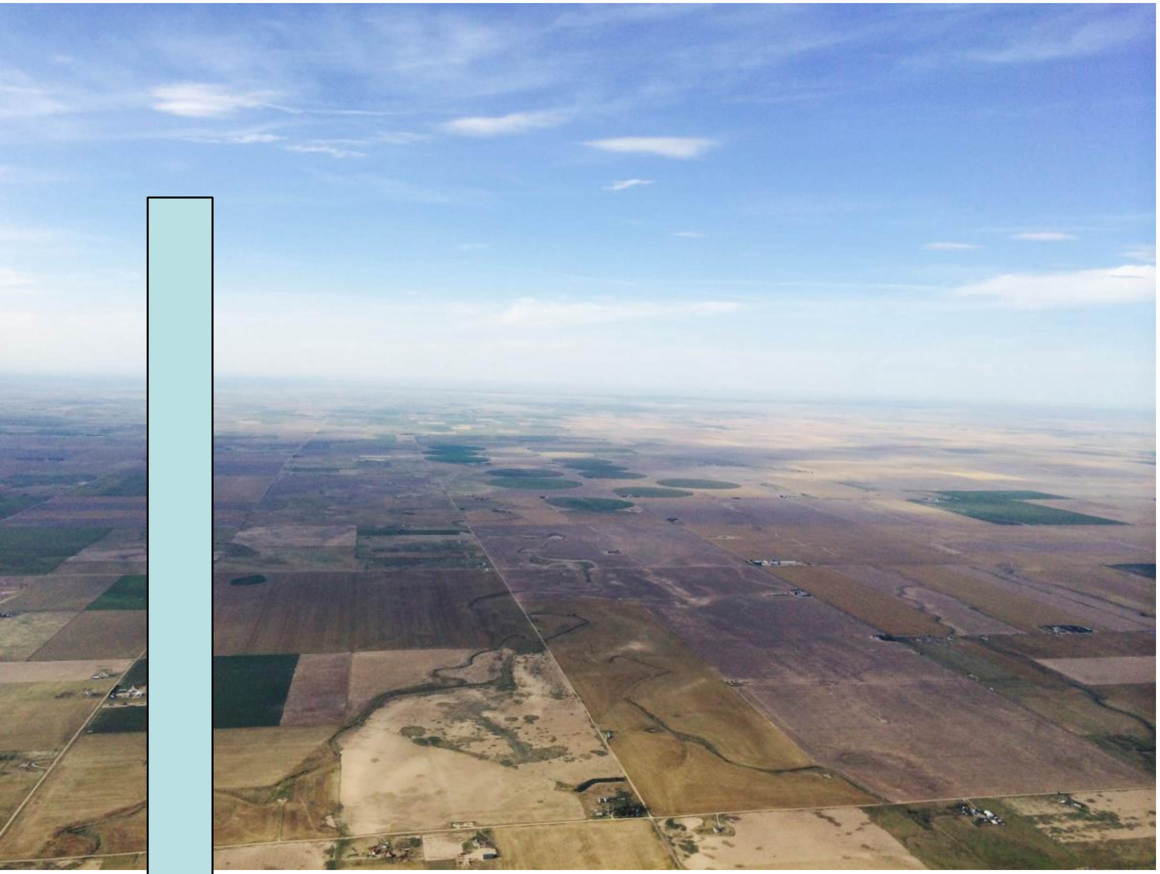


CO_2 utilization – pipe dream or reality?



Current Research on Atmospheric and Captured CO_2 Utilization

Large scale "capture" and use of CO_2



Selectively use CO_2 from the atmosphere directly by natural or artificial photosynthesis; convert to fuels

Capture gases at source, purify CO_2

Low-Energy CO_2 Capture through Cooperative Adsorption

Scientific Achievement

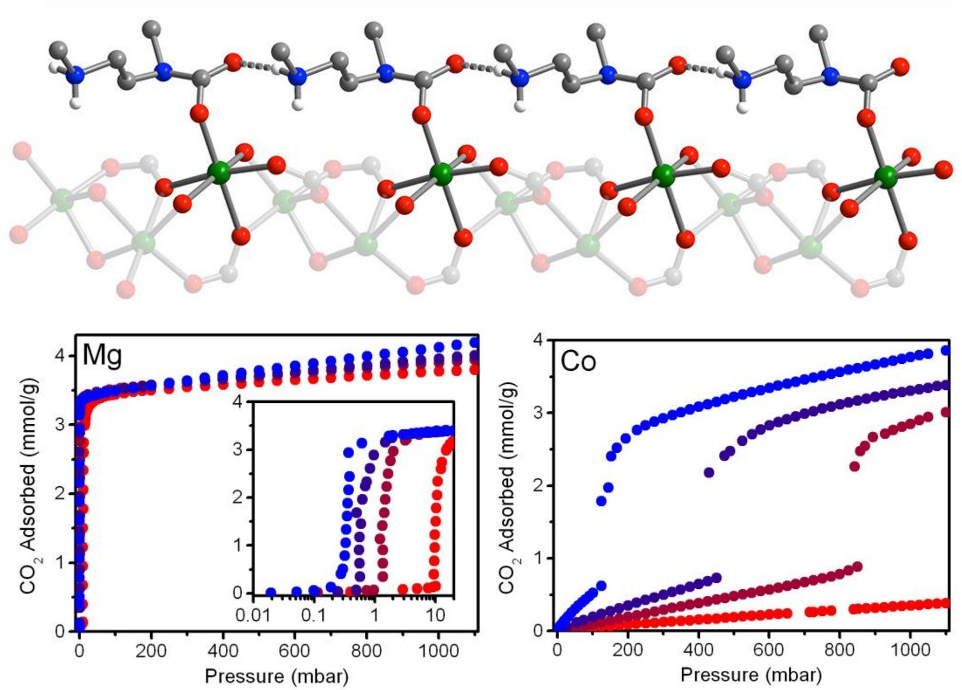
An unprecedented cooperative mechanism for CO_2 capture via insertion into metal–amine bonds is revealed

Significance and Impact

Understanding the mechanism enables us to design new MOF adsorbents that can significantly reduce the energy required for CO_2 capture from a power plant flue gas

Research Details

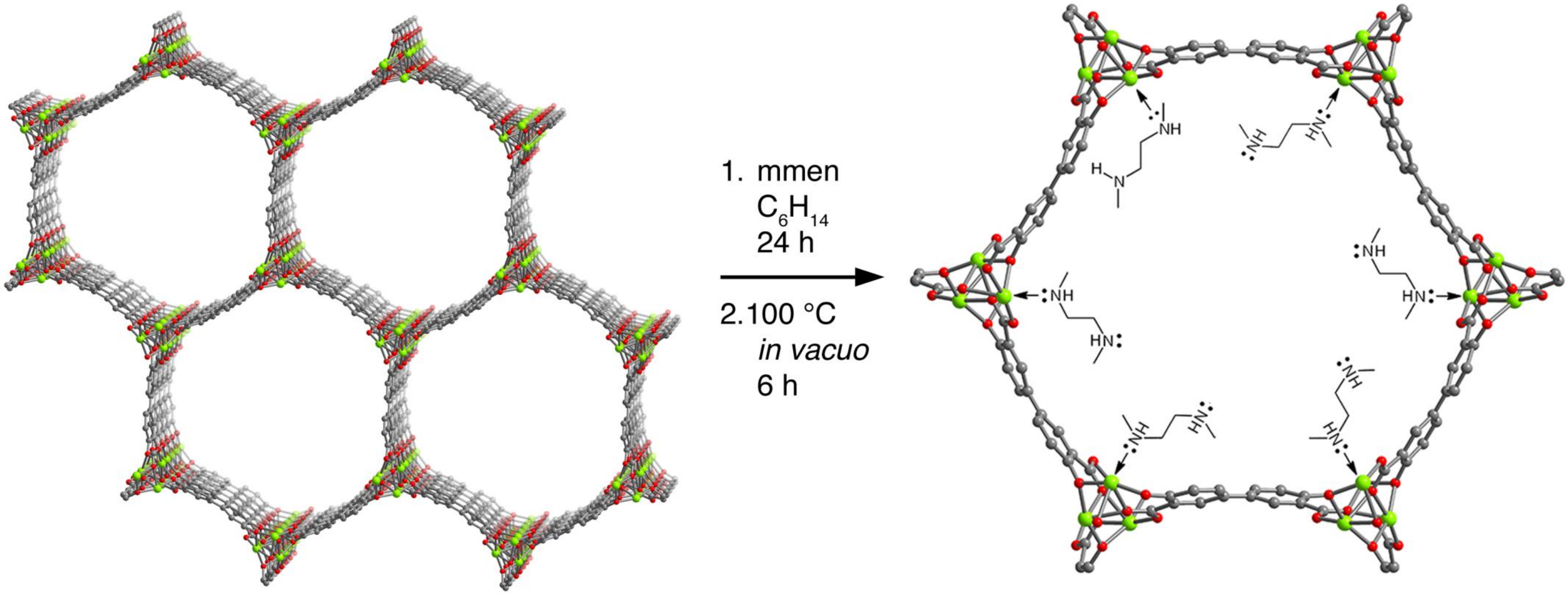
- Insertion of CO_2 at one site facilitates insertion at a neighboring site, leading to formation of ammonium carbamate chains via a chain reaction
- The pressure of the step can be systematically tuned to minimize the energy of CO_2 separations



Top: As revealed by powder x-ray diffraction, CO_2 is adsorbed by mmen-Mn_2(dobpdc) via insertion into metal-amine bonds. One-dimensional chains of ammonium carbamate are formed as the cooperative process propagates along the pore surfaces.
Bottom: CO_2 adsorption isotherms at 25, 40, 50, and 75 °C for mmen-M_2(dobpdc) (M = Mg, Co) show how the position of the step can be controlled by varying metal-amine bond strength.

McDonald, Mason, Kong, Bloch, Gygi, Dani, Crocellà, Giordano, Odoh, Drisdell, Vlaisavljevich, Dzubak, Poloni, Schnell, Planas, Kyuho, Pascal, Prendergast, Neaton, Smit, Kortright, Gagliardi, Bordiga, Reimer, Long
Nature **2015**, http://dx.doi.org/10.1038/nature14327

A Diamine-Appended Metal-Organic Framework

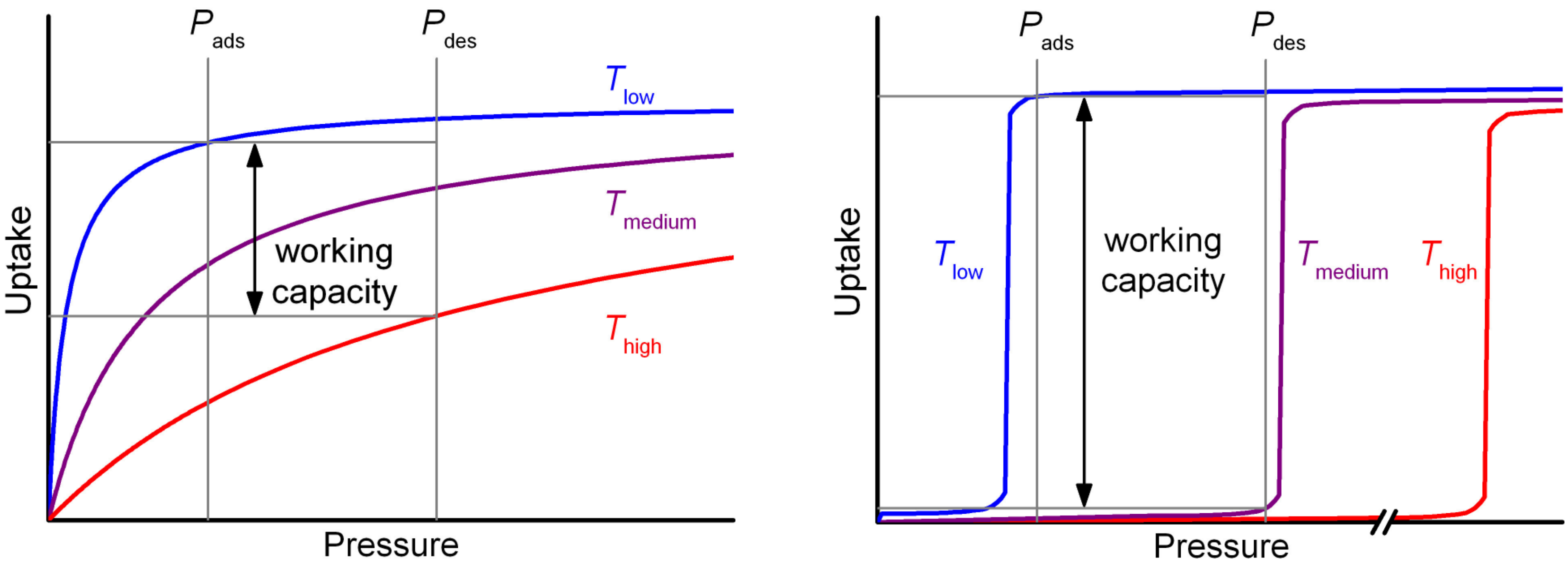


Mg_2(dobpdc) mmen-Mg_2(dobpdc)

- Dangling amines coat the periphery of the channel leaving space for rapid CO_2 diffusion

McDonald, Lee, Mason, Wiers, Hong, Long *J. Am. Chem. Soc.* **2012**, *134*, 7056

Classical versus Phase-Change Adsorbents

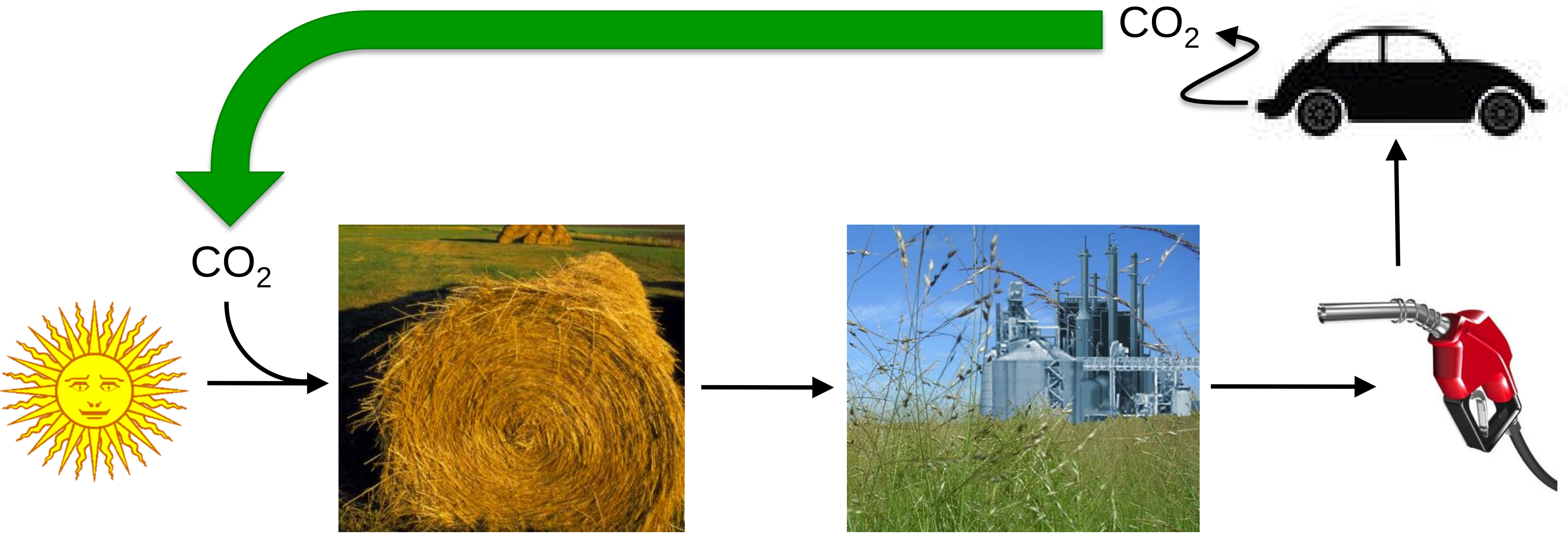


- For phase-change adsorbents, a small change in temperature gives a large working capacity

McDonald, Mason, Kong, Bloch, Gygi, Dani, Crocellà, Giordano, Odoh, Drisdell, Vlaisavljevich, Dzubak, Poloni, Schnell, Planas, Kyuho, Pascal, Prendergast, Neaton, Smit, Kortright, Gagliardi, Bordiga, Reimer, Long *Nature* **2015**, available online

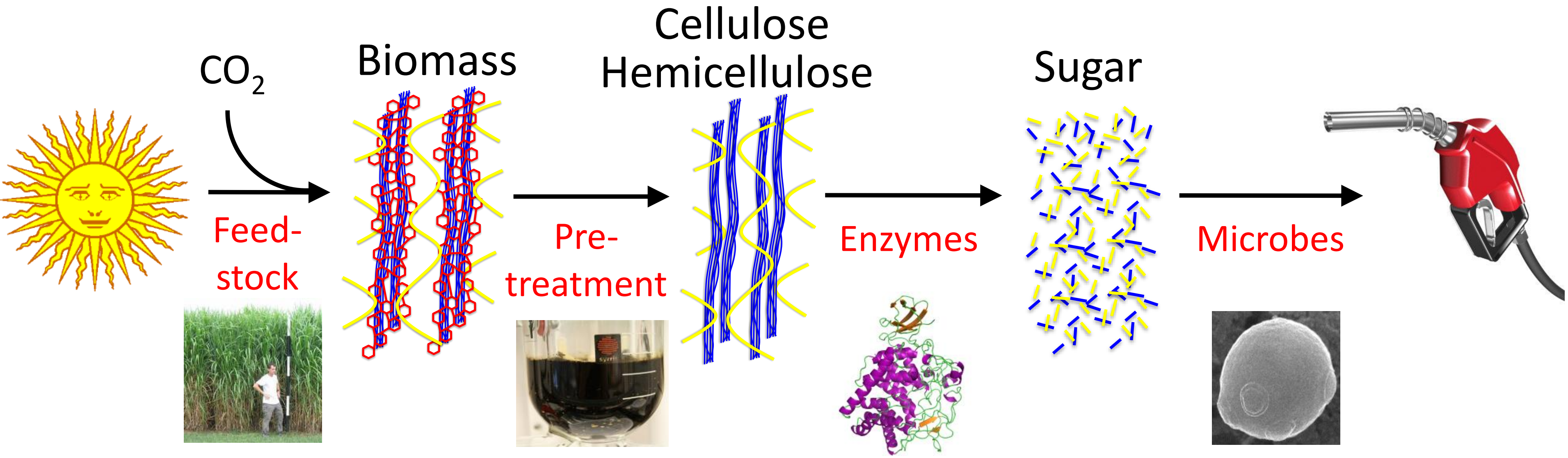
Joint BioEnergy Institute

One of three U.S. Department of Energy-supported National Bio-Energy Research Centers dedicated to enabling clean, carbon-neutral biofuels from cellulosic (non-food) biomass



Berkeley Lab, UC Berkeley, UC Davis, Sandia, LLNL, Carnegie Institution

JOINT BIOENERGY INSTITUTE



JBEI technology development & improvement strategy

Increase C6/C5 ratio	Lower lignin content	Less enzyme use	Lower IL price	Lower IL use	Increase biofuel yield	Increase fermentation productivity

+Lignin valorization

Objective – reduce biofuel cost from current $40 to ca. $3/gal

JBEI's Research Approach is High Risk

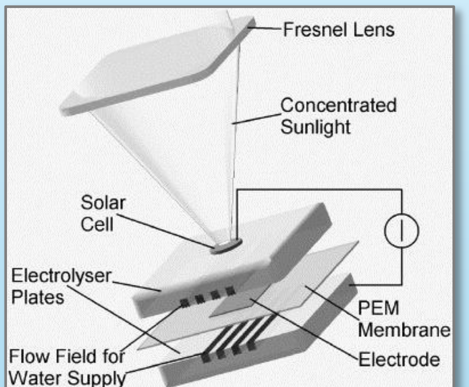
JBEI approach	Less risky approach
Genetically modified crops for optimized for biofuel production	Understanding current crops for use as biofuel feedstocks
Ionic liquid pretreatment process • high yield saccharification of biomass • low levels of inhibitors • lignin valorization	Improvements to existing methods for biomass deconstruction
Microbes engineered to produce **drop-in fuels** for all transportation segments	Incremental improvements in production costs of existing fuels (ethanol, butanol)

Joint Center for Artificial Photosynthesis (JCAP)

Aims to develop an efficient, scalable and robust prototype that generates fuel from sunlight, water, and carbon dioxide.

Types of Artificial Photosynthesis Devices

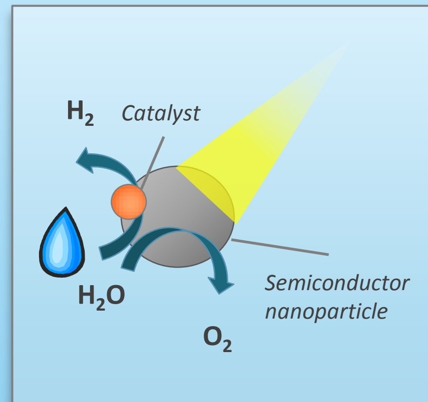
Photovoltaic + Electrolyzer



Advantages: Efficient and already developed

Challenges: Expensive

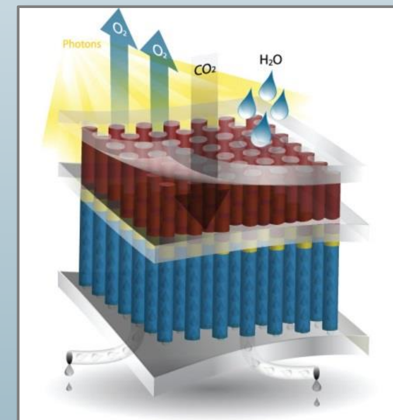
Particle Dispersions



Advantages: Low cost

Challenges: Dangerous

Integrated System

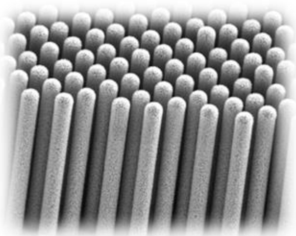


Advantages: Efficient and safe; potentially low cost
Challenges: Earth-abundant materials undiscovered

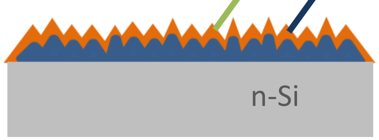
JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

Joint Center for Artificial Photosynthesis

Science



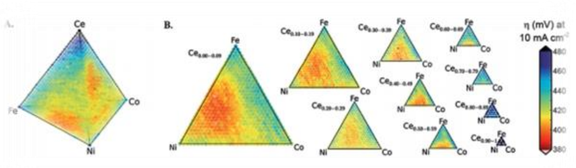
Efficient TiO_2-protected amorphous Si photo-cathodes demonstrated



Stabilization of efficient earth-abundant photo-anodes at extreme pH by nanotexturing and catalyst overcoat

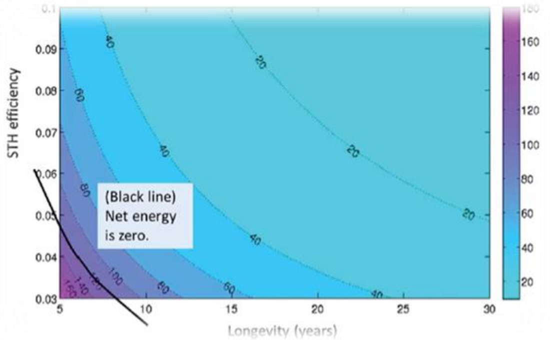
Caltech, Berkeley plus other partners

Discovery and demon-stration of new class of NiFeCoCe oxygen evolu-tion catalyst



Prototypes & devices

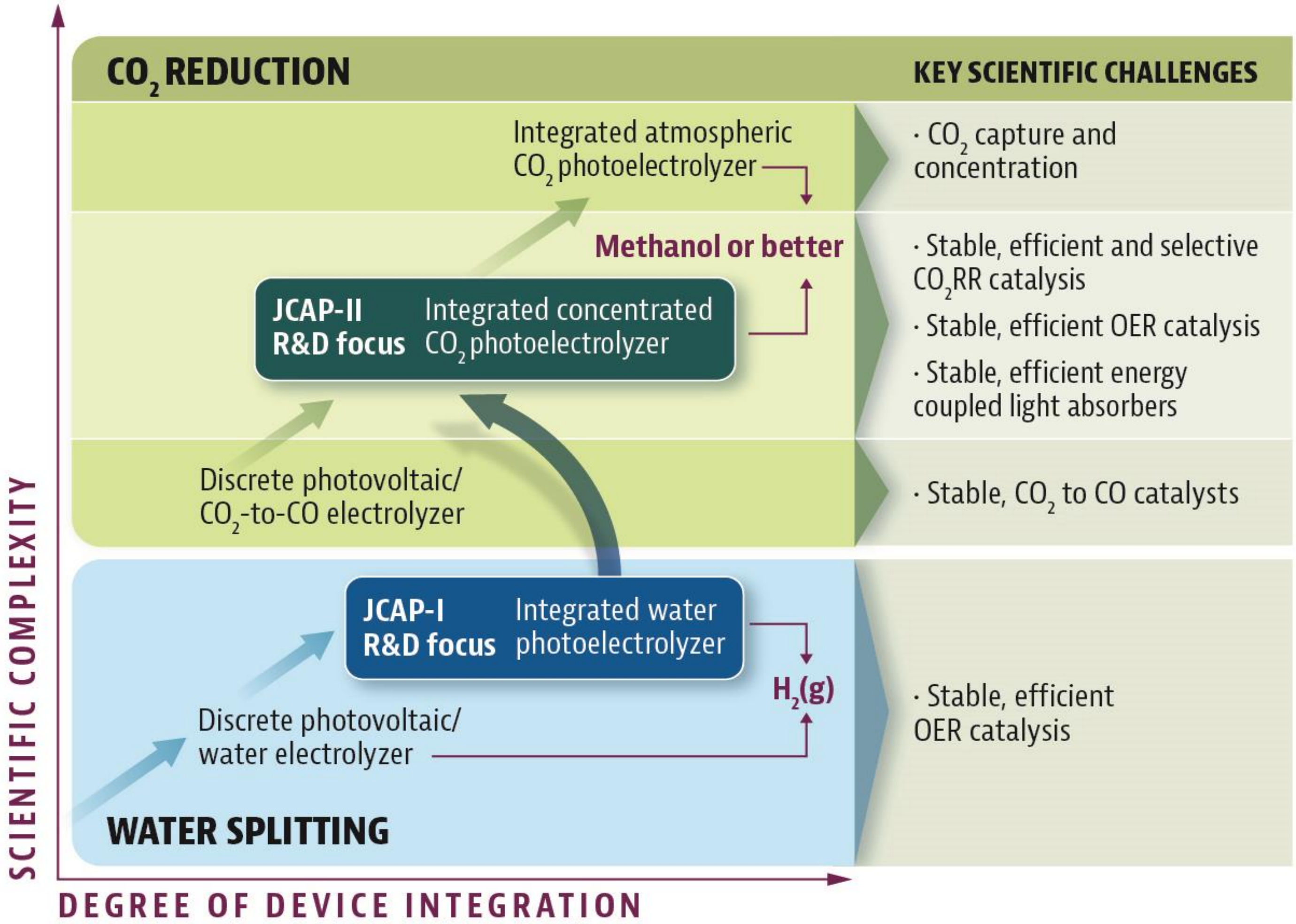
Solar fuels generator demonstrated at neutral pH by electrolyte recirculation



Energy efficiency tradeoff between panel lifetime and device efficiency determined

JCAP Trajectory in Initial Phase and Renewal

JCAP transitions to the the challenge of progress toward a solar fuels generator producing fuel from carbon dioxide, sunlight and water.



JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

JCAP RESEARCH THRUSTS

1 THRUST 1 Electrocatalysis

KEY SCIENTIFIC GAP

Understanding the structural and compositional parameters that govern the:

· Activity and selectivity of CO_2RR catalysis, and
· Activity and selectivity of OER catalysis

KEY FOCUS

· Discovery and understanding of heterogeneous CO_2RR electrocatalysis
· Discovery and understanding of heterogeneous OER electrocatalysis

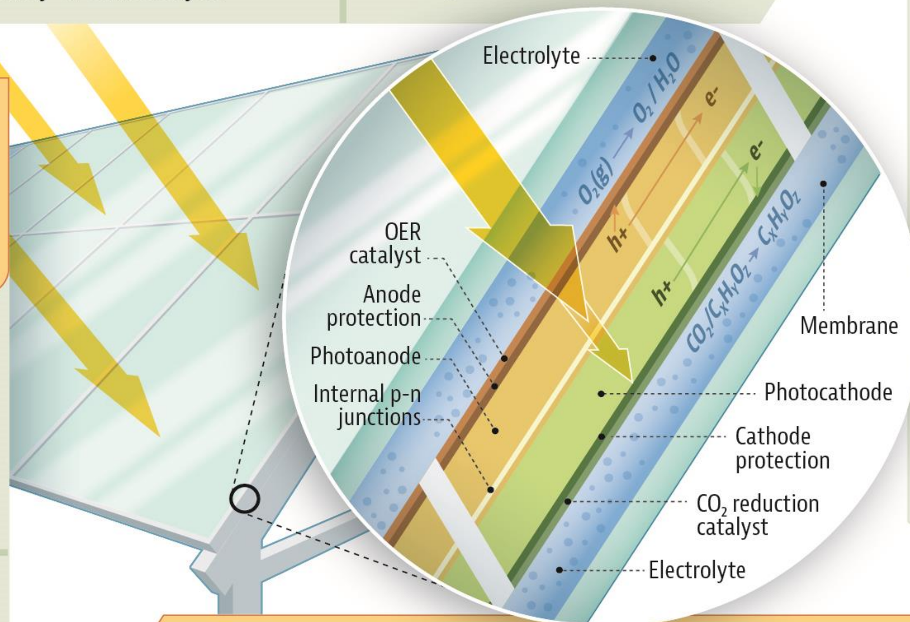
2 THRUST 2 Photocatalysis and light capture

KEY SCIENTIFIC GAP

Understanding the effect of **(1)** surface composition, **(2)** surface structure, and **(3)** electronic structure on the photocatalytic activity for CO_2RR and OER

KEY FOCUS

· Discovery and undertsanding of CO_2RR and OER photocatalysis.
· Development and understanding of light harvesting photonic architectures



4 THRUST 4 Modeling, test-bed prototyping, & benchmarking

KEY SCIENTIFIC GAP

Understanding of how charge-and-ion-transport through components affects the efficiency of integrated devices

KEY FOCUS

· Modeling and simulation of device parameters and test-bed architectures
· Development and understanding of light harvesting photonic architectures

3 THRUST 3 Materials integration into components

KEY SCIENTIFIC GAP

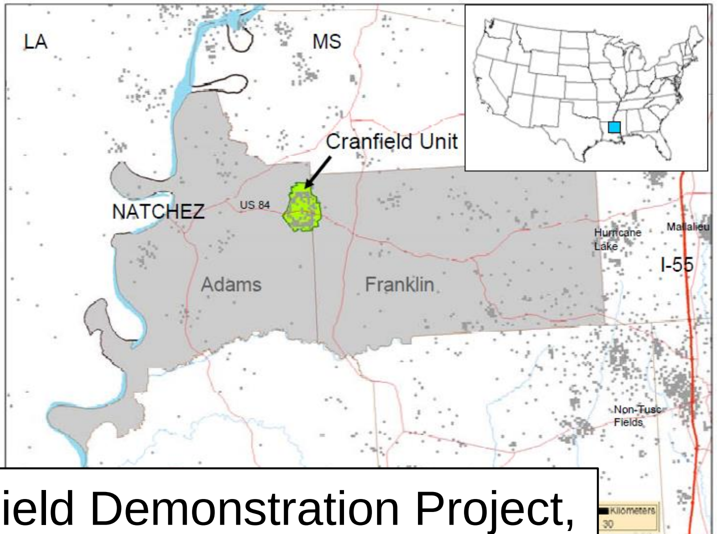
Understanding of how interfacial phenomenon influence:

· Light absorption and generation efficiency
· (Photo)electrocatalytic activity

KEY FOCUS

· Development and understanding of integrated catalyst/light absorber assemblies

Engineered Geothermal Systems with $scCO_2$ as the working fluid phase



Field Demonstration Project,
Cranfield Mississippi
B. Freifeld, LBNL

- **Heat extraction** rates with CO_2 are ≈50 % larger than for water.
- CO_2 is favorable in terms of **wellbore hydraulics**.
- Rock-fluid **chemical interactions** are weaker for dry, anhydrous CO_2 than for water.
- **Fluid losses** are costly for water, but could earn greenhouse gas storage credits for CO_2.

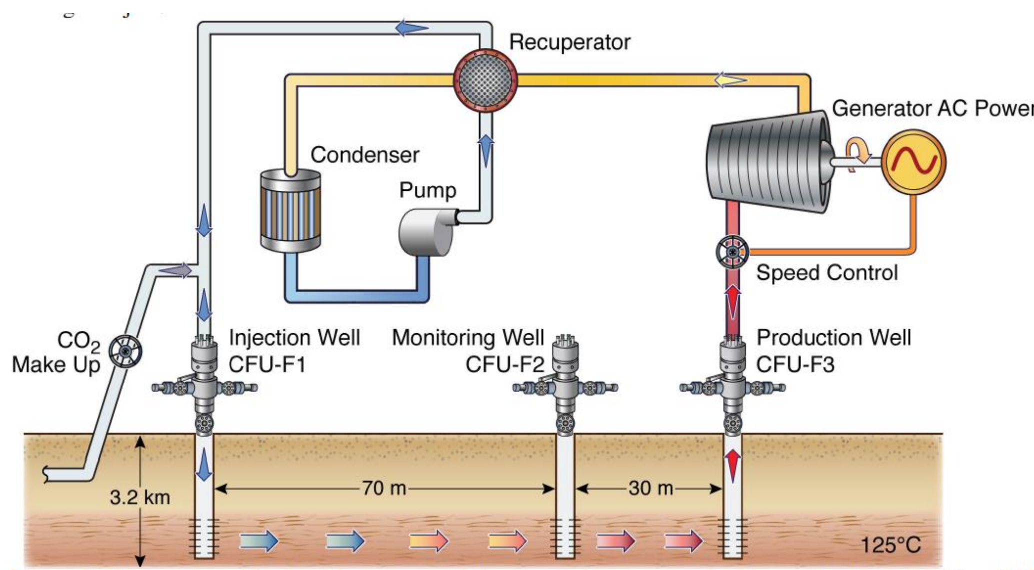


Figure 1. Proposed combined CO2 storage pilot/geothermal energy production at the SECARB Cranfield DAS demonstration site.

Summary

- Geologic carbon storage is necessary to get through the next 150 years with acceptable total carbon emissions
- Using CO_2 in large enough quantities to make a difference in emissions is challenging, but…
- Making fuels from sunlight and CO_2 is one way to do it – either with natural photosynthesis (cellulosic biofuels) or through artificial photosynthesis.
- EOR with supercritical captured anthropogenic CO_2 can contribute some reduction in carbon intensity in the next few decades
- Other possibilities, like Engineered Geothermal Systems (EGS) with $scCO_2$ are at early stages of evaluation

Taylor Glacier, Antarctica

Thank you

BERKELEY LAB · OAK RIDGE National Laboratory · THE OHIO STATE UNIVERSITY · PURDUE UNIVERSITY · Washington University in St. Louis School of Engineering & Applied Science