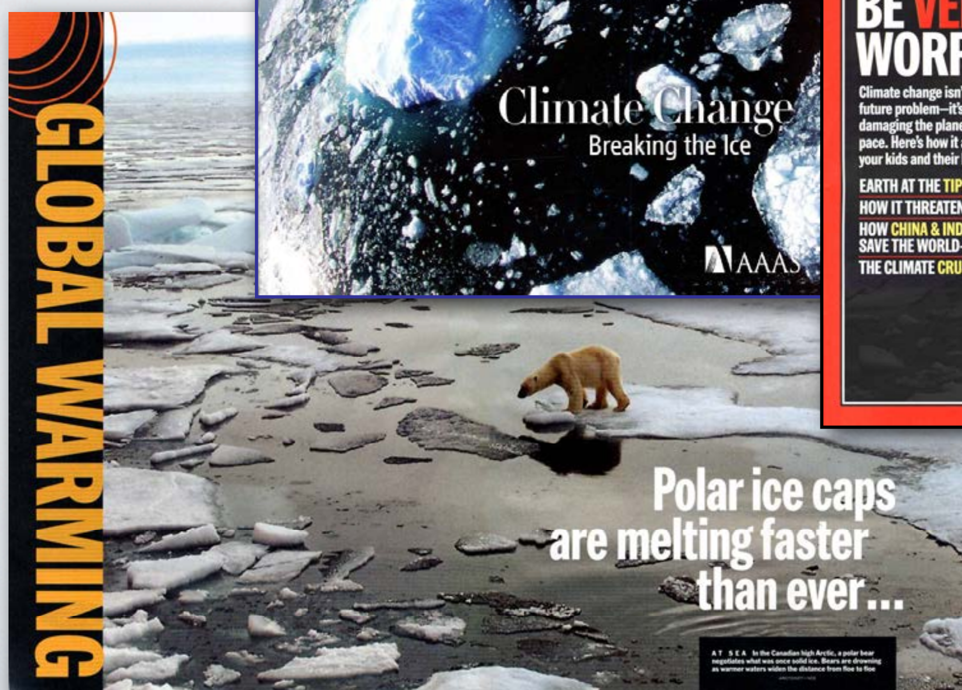
The Mathematics Behind Energy and Earth Systems Modeling

Juan Meza
Department Head, Senior Scientist
Lawrence Berkeley National Laboratory

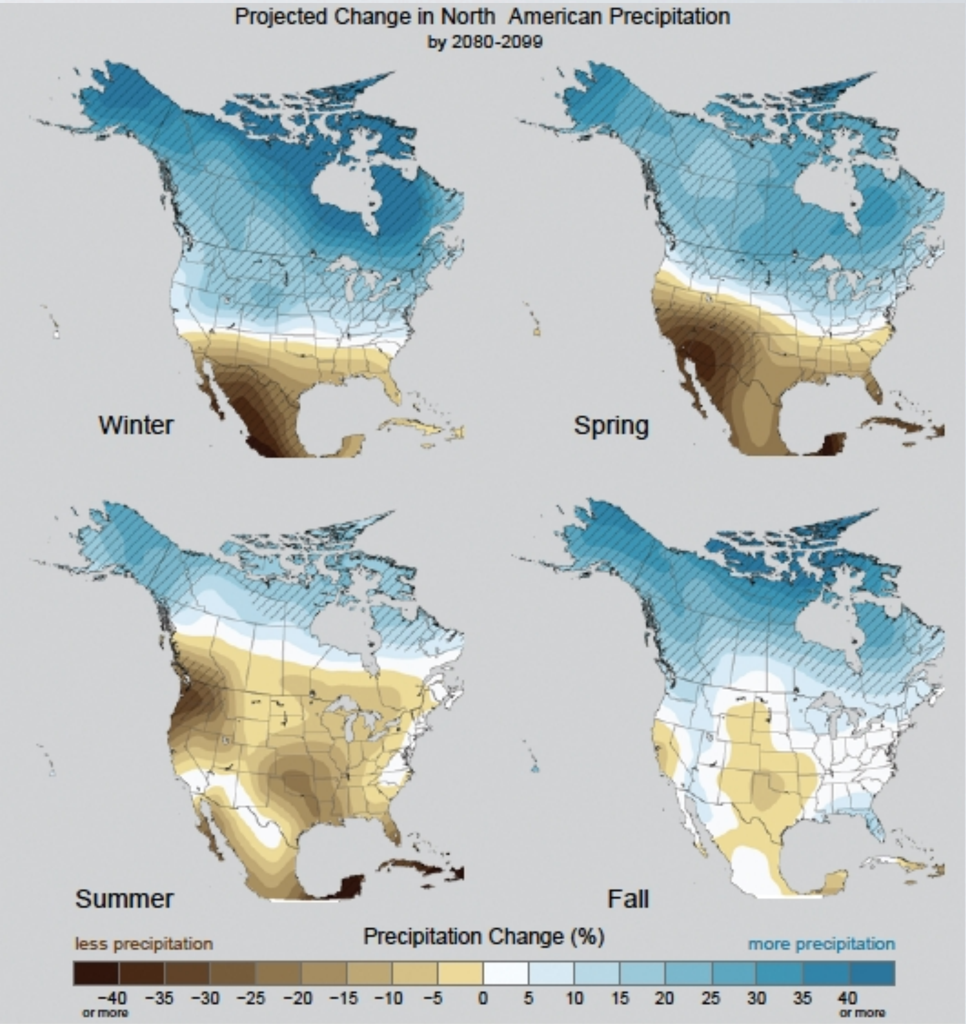
SIAM Annual Meeting, Denver, CO, July 6-10, 2009

CLIMATE CHANGE IS BIG NEWS

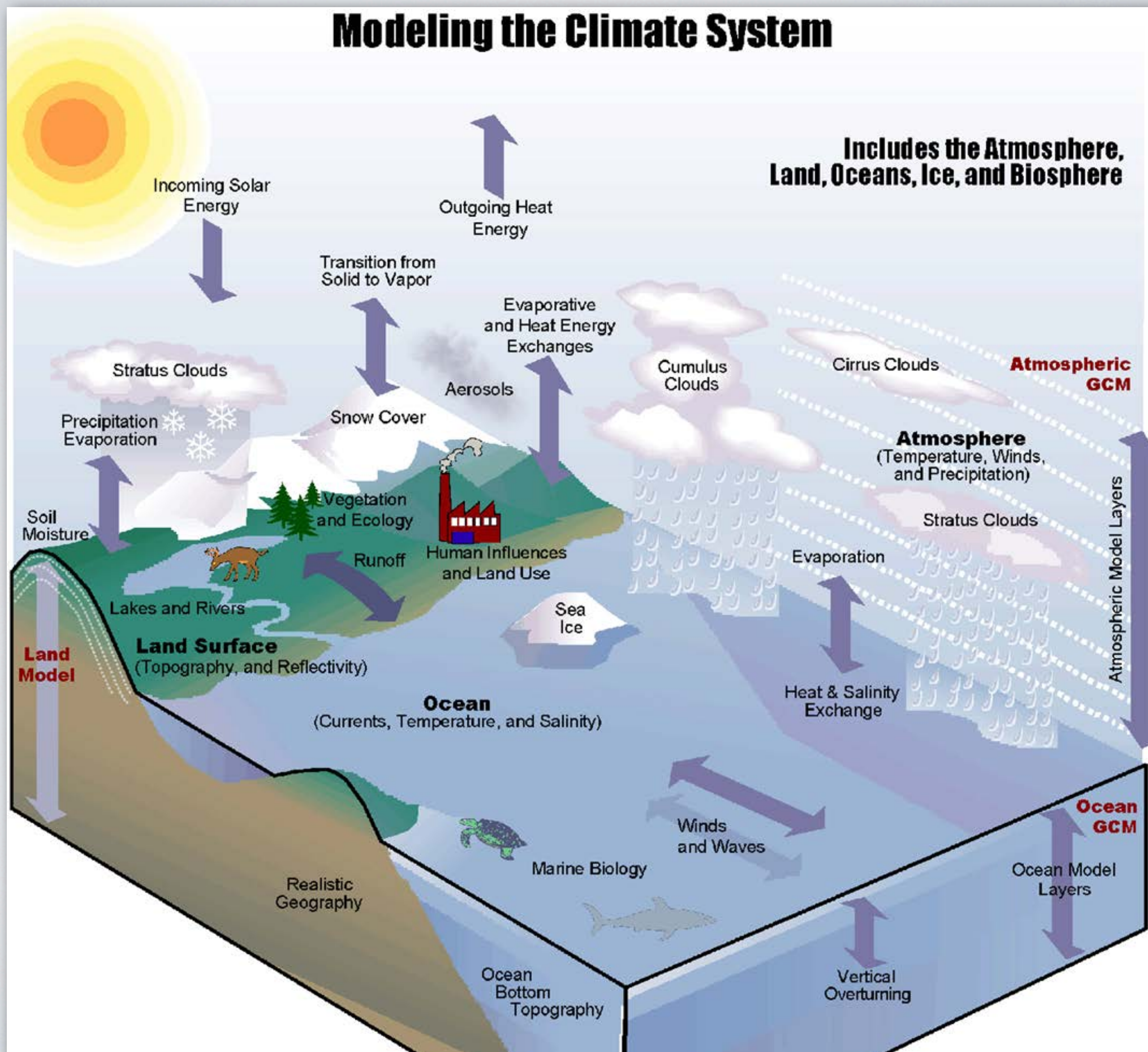


KEY FINDINGS

1. Global warming is unequivocal and primarily human-induced.
2. Climate changes are underway in the United States and are projected to grow.
3. Widespread climate-related impacts are occurring now and are expected to increase.
4. Climate change will stress water resources.
5. Crop and livestock production will be increasingly challenged.
6. Coastal areas are at increasing risk from sea-level rise and storm surge.
7. For more information see: www.globalchange.gov

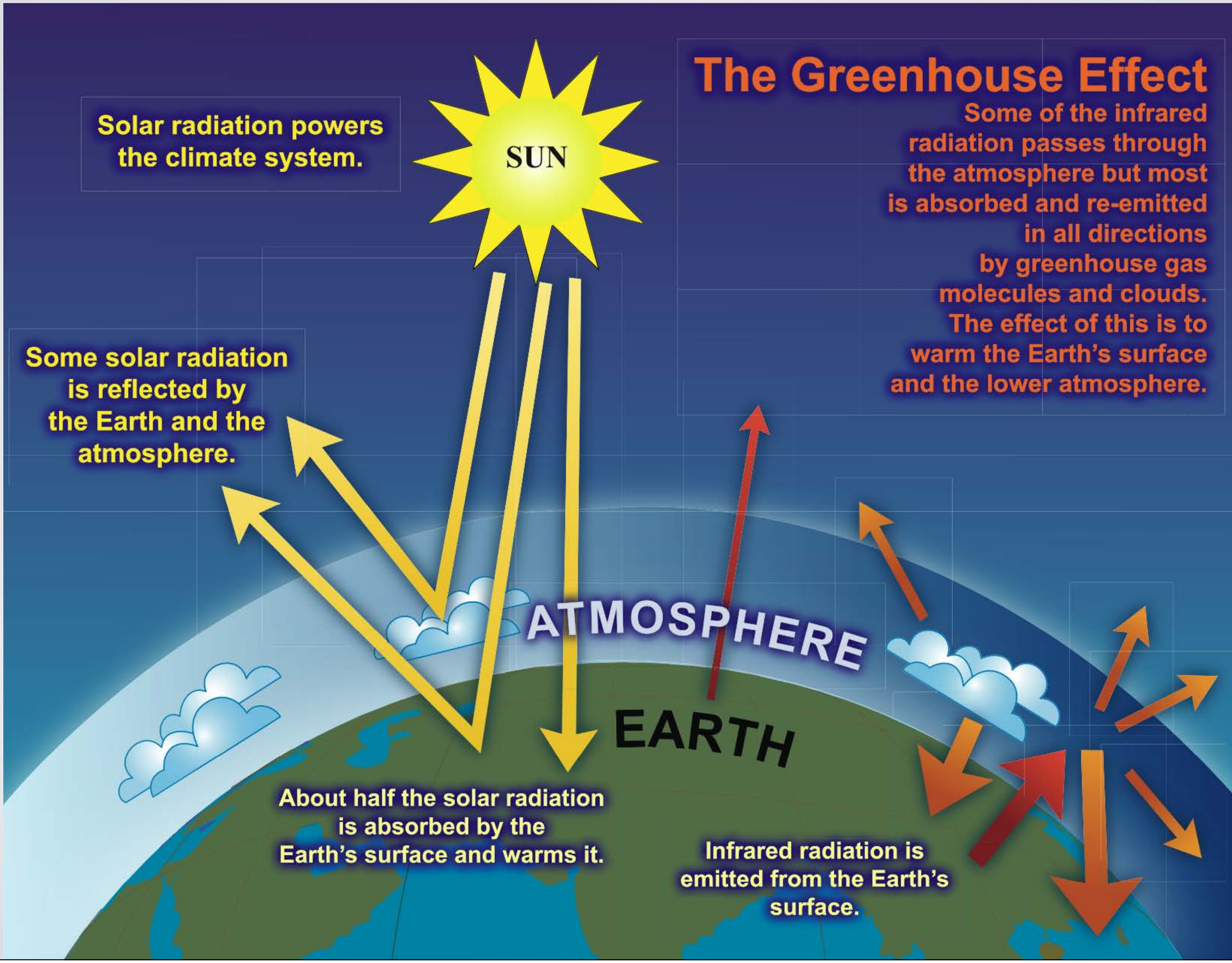


Global Climate Change Impacts in the United States, Thomas R. Karl, Jerry M. Melillo, and Thomas C. Peterson, (eds.). Cambridge University Press, 2009.



Modeling the Climate System
Includes the Atmosphere, Land, Oceans, Ice, and Biosphere
Incoming Solar Energy
Outgoing Heat Energy
Transition from Solid to Vapor
Evaporative and Heat Energy Exchanges
Stratus Clouds
Aerosols
Cumulus Clouds
Cirrus Clouds
Atmospheric GCM
Precipitation Evaporation
Snow Cover
Atmosphere (Temperature, Winds, and Precipitation)
Soil Moisture
Vegetation and Ecology
Stratus Clouds
Runoff
Human Influences and Land Use
Evaporation
Atmospheric Model Layers
Lakes and Rivers
Sea Ice
Land Model
Land Surface (Topography, and Reflectivity)
Heat & Salinity Exchange
Ocean (Currents, Temperature, and Salinity)
Ocean GCM
Winds and Waves
Marine Biology
Ocean Model Layers
Realistic Geography
Ocean Bottom Topography
Vertical Overturning

GREENHOUSE EFFECT



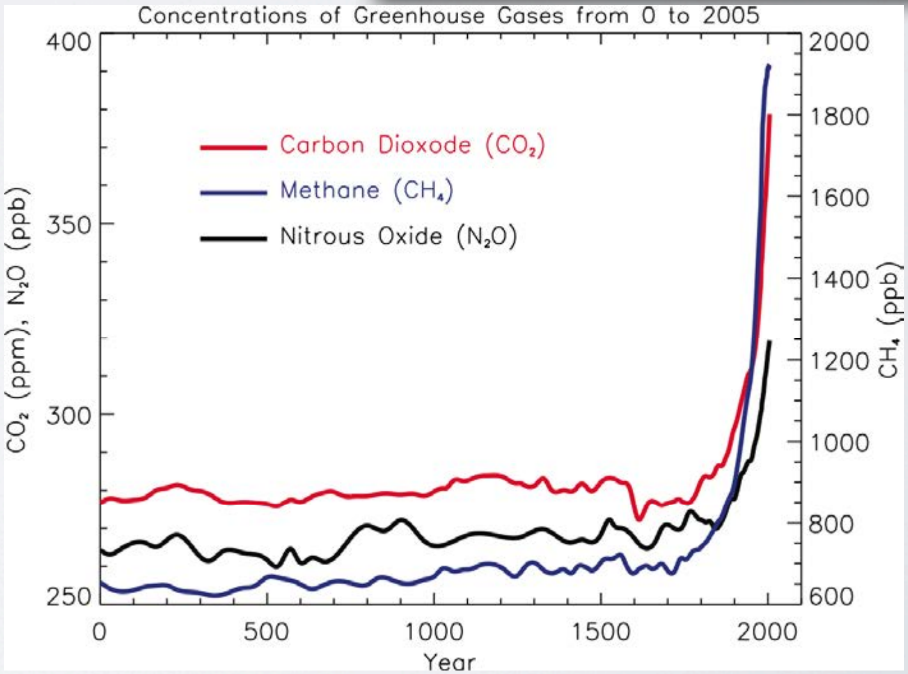
FIRST MENTION OF GREENHOUSE EFFECT

- Developed mathematical theory for the temperature of the terrestrial globe
- "*The temperature [of the Earth] can be augmented by the interposition of the atmosphere, because heat in the state of light finds less resistance in penetrating the air, than in repassing into the air when converted into non-luminous heat*"
- General Remarks on the Temperature of the Terrestrial Globe and the Planetary Spaces (1824)

JEAN BAPTISTE JOSEPH FOURIER

ANNUAL GLOBAL RELEASE OF CO_2 IS 27 BILLION TONS

- In US, combustion
  - Transportation
  - Power generation
- 40% coal, 40% oil, 20% natural gas
- US consumes (per day):
  - 20 million barrels of oil
  - 60 billion cubic feet natural gas
  - 3 million tons of coal



Climate Change 2007, The Physical Science Basis, Working Group 1, Solomoon, Qin, Manning ed.

WE'LL CONSIDER THREE AREAS WHERE MATH, ENERGY, AND CLIMATE INTERSECT

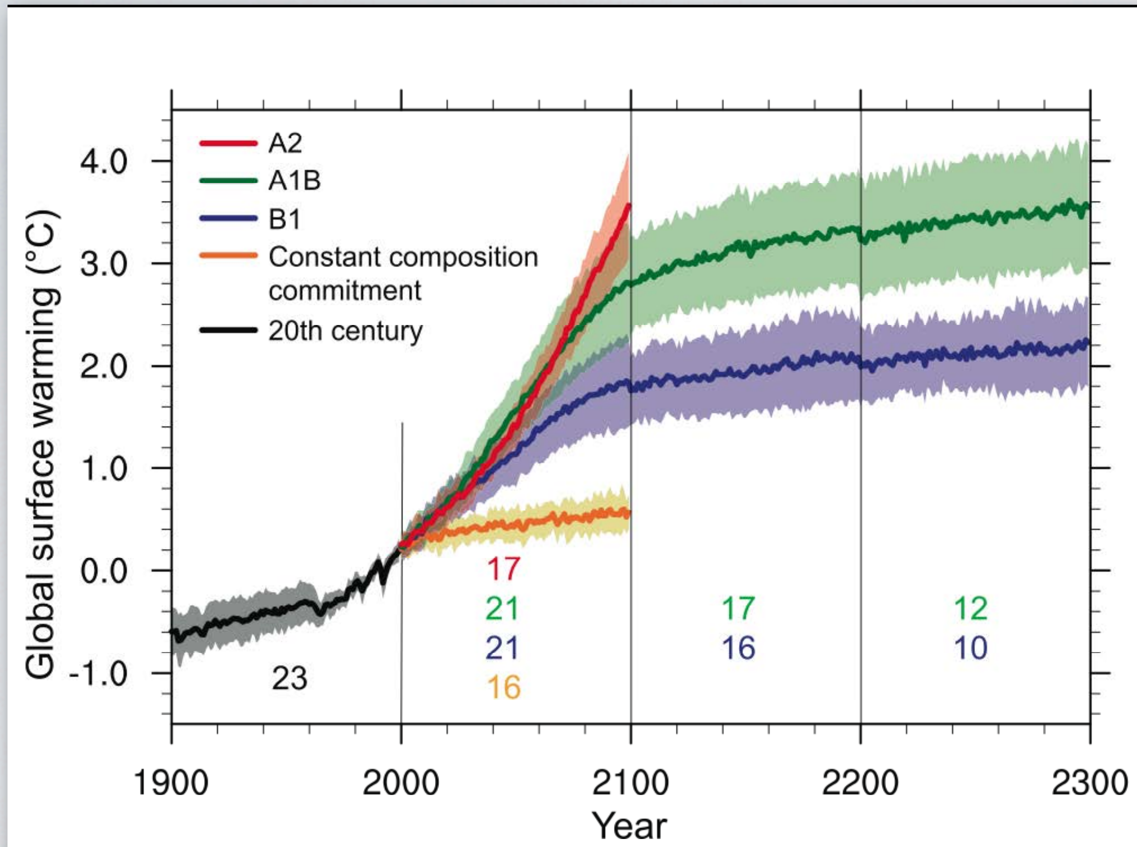


Figure 10.4

- What can we say about our future climate and its effects on us?
- What are we doing today to improve our use of energy?
- What can we do to change how we use energy in the future?

http://ipcc-wg1.ucar.edu/wg1/wg1_home.html

WHAT CAN WE SAY ABOUT OUR FUTURE CLIMATE AND ITS EFFECTS ON US?

PRIMITIVE EQUATIONS FOR ATMOSPHERE

LEWIS FRY RICHARDSON

$$\frac{du}{dt} - \left(f + u\frac{\tan\phi}{a}\right)v = -\frac{1}{a\cos\phi}\frac{1}{\rho}\frac{\partial p}{\partial \lambda} + F_\lambda$$

$$\frac{dv}{dt} + \left(f + u\frac{\tan\phi}{a}\right)u = -\frac{1}{\rho a}\frac{\partial p}{\partial \phi} + F_\phi$$

$$g = -\frac{1}{\rho}\frac{\partial p}{\partial z}$$

momentum

$$\frac{\partial \rho}{\partial t} = -\frac{1}{a\cos\phi}\left[\frac{\partial}{\partial \lambda}(\rho u) + \frac{\partial}{\partial \phi}(\rho v\cos\phi)\right] - \frac{\partial}{\partial z}(\rho w)$$

mass

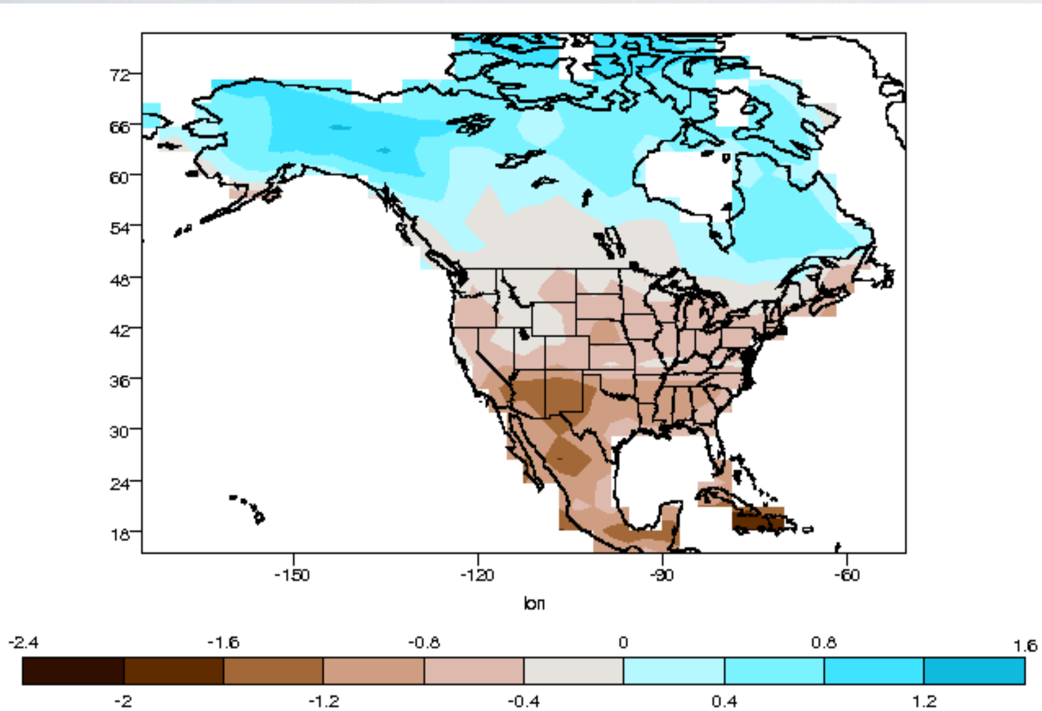
$$C_p\frac{dT}{dt} - \frac{1}{\rho}\frac{dp}{dt} = Q$$

energy

$$p = \rho RT$$

equation of state

DROUGHT CONDITIONS INCREASE IN SW US AND MEXICO



Drought —— Flood

The predicted average value of PDSI in 2090 using the 1950-1999 period as a reference. Analysis of 22 models contributed to IPCC AR4 database

M.F. Wehner (LBNL) et al. work in progress

- Most of SW US and Mexico would be in drought, while most of Canada would be in flood conditions
- Precipitation decreases in the Southwest and increases substantially in the Northern latitudes
- This assumes that the CO_2 content of the atmosphere stabilizes to 720ppm in the middle of the 22nd century

THE GENERALIZED EXTREME VALUE (GEV) DISTRIBUTION CAN BE USED TO STUDY CLIMATE

$$F(x) = \begin{cases} e^{-[1+\xi(x-\mu)/\sigma]^{-1/\xi}} & , \quad \xi \neq 0 \\ e^{-e^{-(x-\mu)/\sigma}} & , \quad \xi = 0 \end{cases}$$

$$\text{where} \quad \mu = \text{location}, \sigma = \text{scale}, \xi = \text{shape}$$

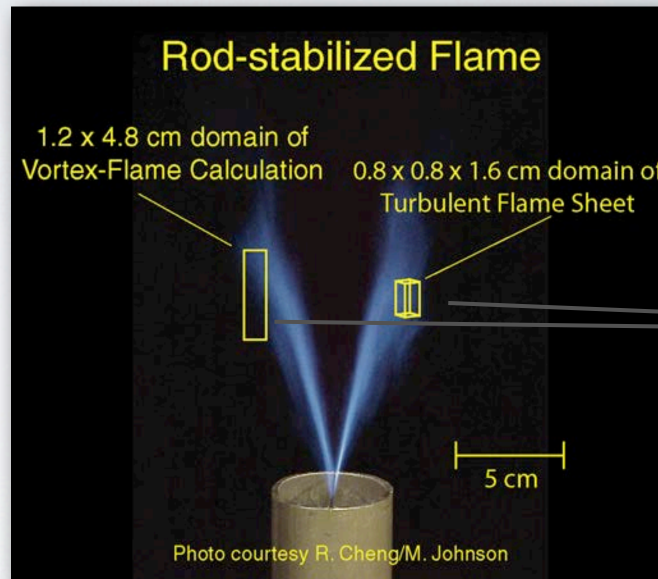
The return value of a random variable, X_T is that value that is exceeded, on average, once in a period of time, T

$$X_T = \begin{cases} \mu + \sigma[1 - \{-ln(1 - 1/T)\}^{-\xi}/\xi & , \quad \xi \neq 0 \\ \mu - \sigma[ln(-ln(1 - 1/T)) & , \quad \xi = 0 \end{cases}$$

WHAT ARE WE DOING TODAY TO IMPROVE OUR USE OF ENERGY?

INCREASING COMBUSTION EFFICIENCY IS IMPORTANT IN REDUCING GREENHOUSE GASES

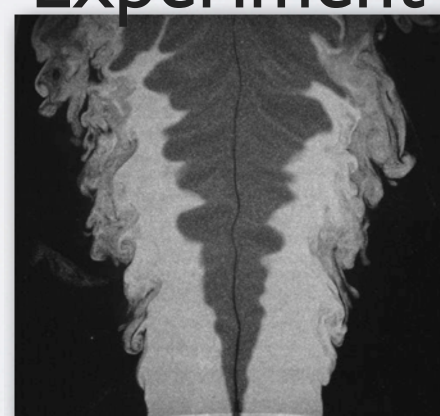
- Most new systems are based on lean premixed turbulent combustion because they have potentially high-efficiency and low emissions
- Challenges to system design
  - Natural flame instabilities
  - Sensitivity to fuel
- Advances in applied mathematics have dramatically increased our simulation capability



Before

Simulation

Experiment



LOW MACH NUMBER EQUATIONS

$$\rho \frac{DU}{Dt} = -\nabla\pi + \nabla\cdot\tau$$ ***momentum***

$$\frac{\partial \rho Y_m}{\partial t} + \nabla\cdot(\rho U Y_m) = \nabla\cdot(\rho D_m \nabla Y_m) + \dot{\omega}_m$$ ***species***

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho U) = 0$$ ***mass***

$$\frac{\partial \rho h}{\partial t} + \nabla\cdot(\rho h U) = \nabla\cdot(\lambda\nabla T) + \sum_m \nabla\cdot(\rho h_m D_m \nabla Y_m)$$ ***energy***

Y_m mass fraction

$\dot{\omega}_m$ species production, $\sum \dot{\omega}_m = 0$

h enthalpy, $h = \sum Y_m h_m(T)$

Equation of State $p_0 = \rho RT \sum Y_m / W_m$ ***equation of state***

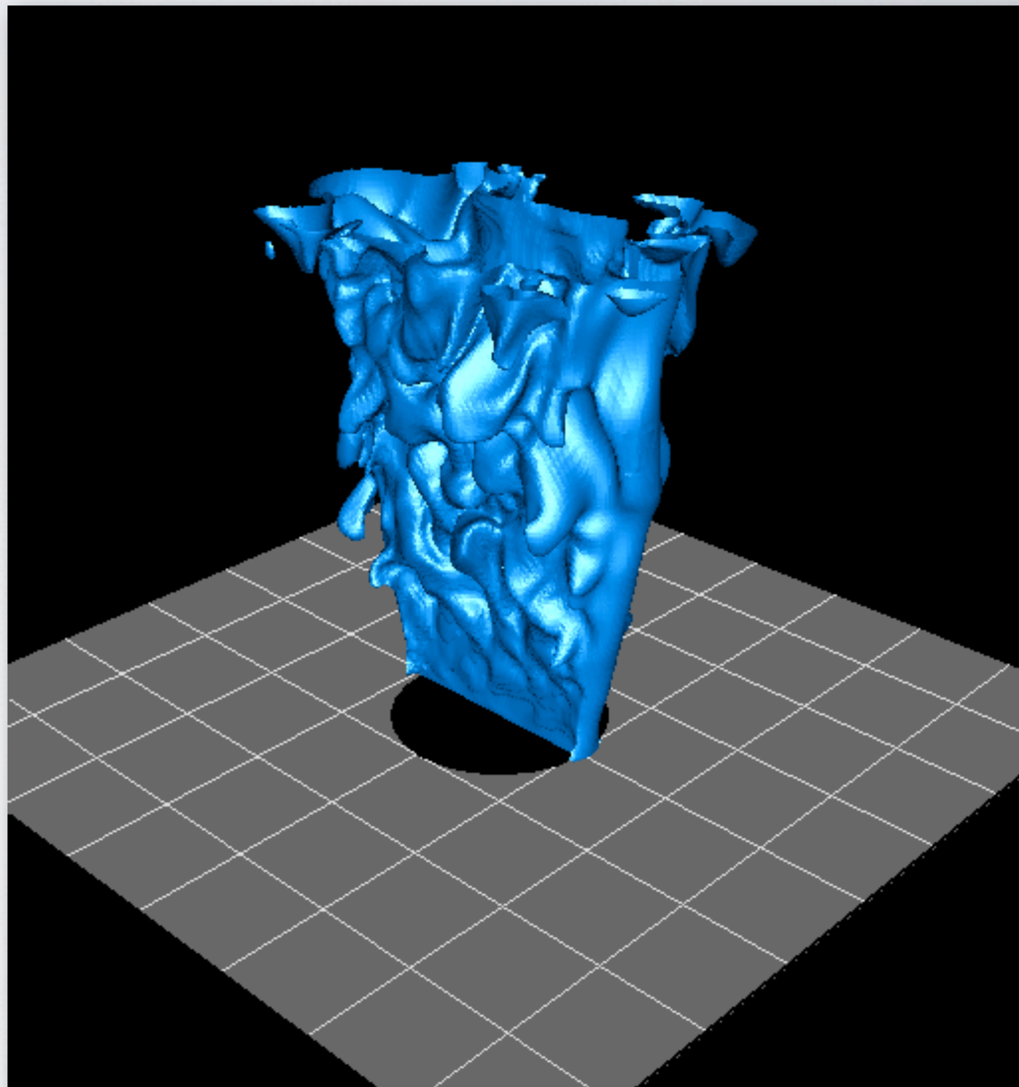
(J.B. Bell, CCSE, LBNL)

MATHEMATICS GROUP INCREASED SIMULATION CAPABILITY BY A FACTOR OF 10,000

Experimental Turbulent V-Flame

(photo courtesy R. K. Cheng, LBNL)

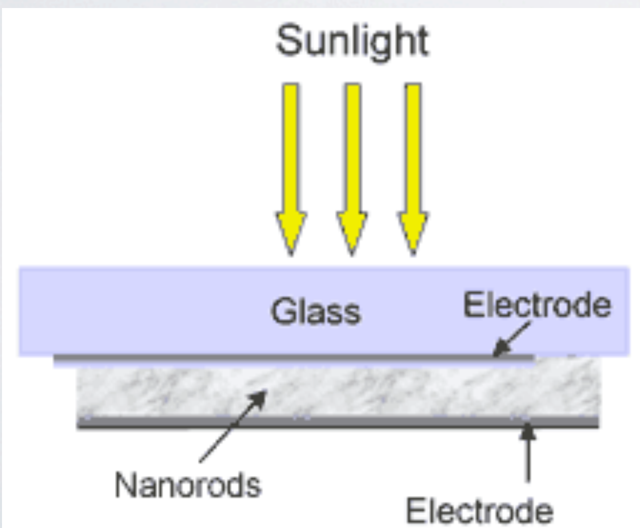
Calculations



(J.B. Bell, CCSE, LBNL)

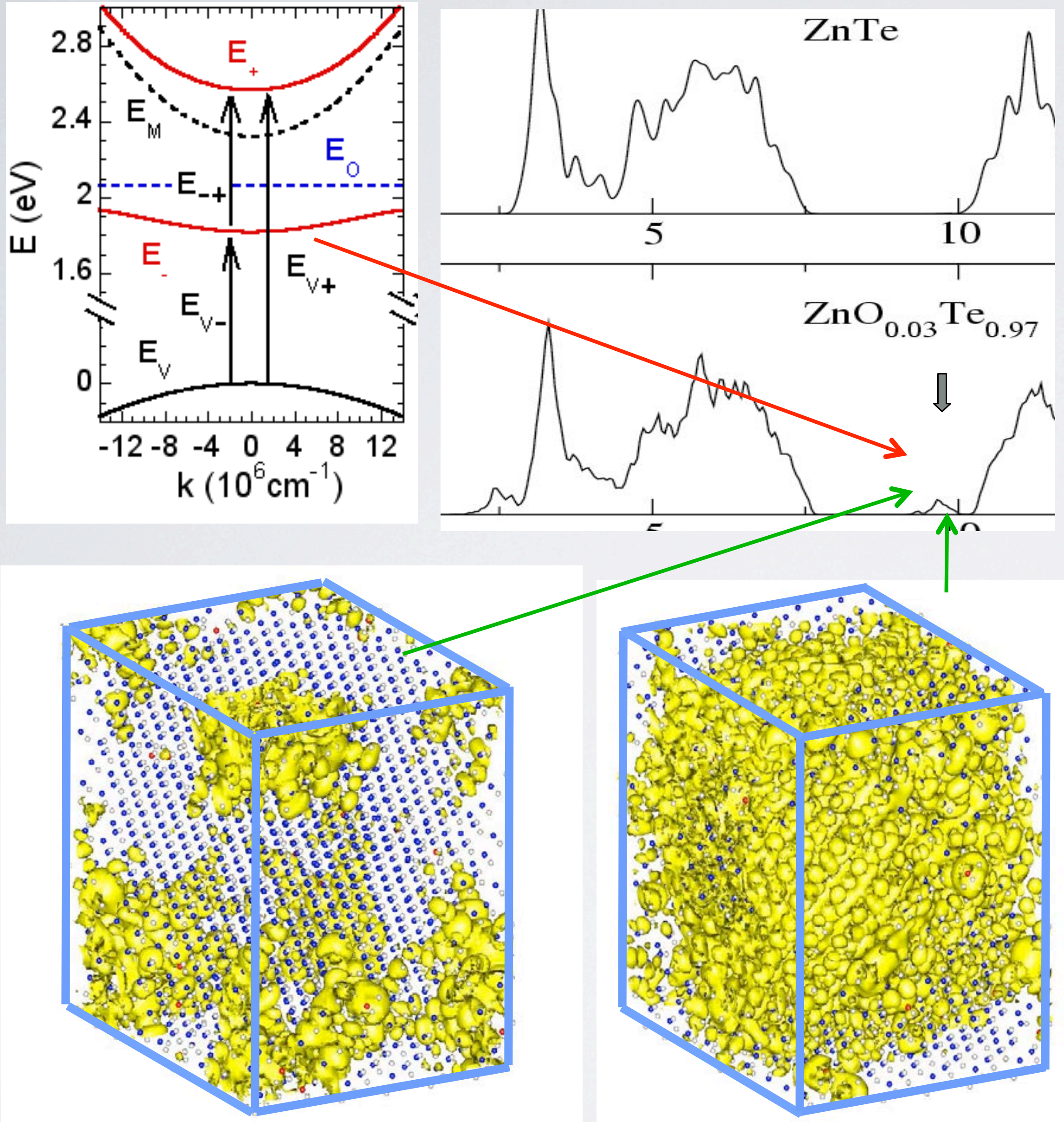
WHAT CAN WE DO TO CHANGE HOW WE USE ENERGY IN THE FUTURE?

PHOTOVOLTAIC SOLAR CELLS



- Solar cells based on inorganic nanorods and semiconducting polymers
- Nanorods can be made of CdSe, a semiconducting material
- Nanorods act like wires, absorbing light and generating hole-electron pairs
- Biggest challenge is cost, ~30 cents/kWh

CAN ONE USE AN INTERMEDIATE STATE TO IMPROVE SOLAR CELL EFFICIENCY?



Highest O induced state *ZnTe bottom of cond. band state*

- Single band material theoretical PV efficiency is 30%
- With an intermediate state, the PV efficiency could be 60%
- One proposed material ZnTe:O – Is there really a gap?
- LS3DF calculation for 3500 atom 3% O alloy [one hour on 17,000 cores of Franklin]
- Yes, there is a gap, and O induced states are very localized.

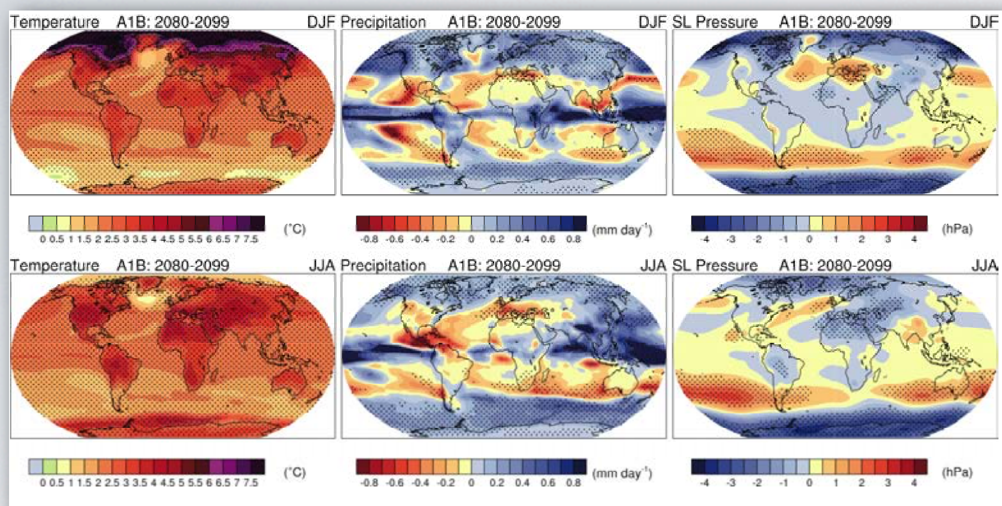
INCITE project, NERSC, NCCS.

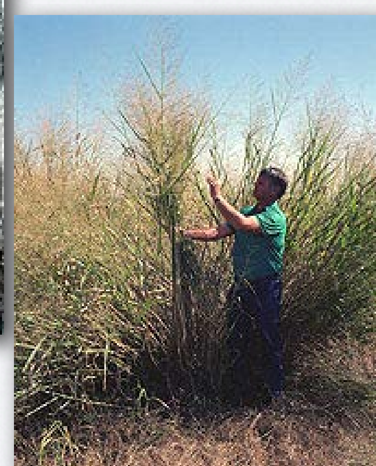
SUMMARY

- Climate change and energy will become increasingly important areas for study
- Modeling and simulation can be used to understand and predict climate change and energy alternatives
- Mathematics is the foundation for climate and energy models.

Many challenges remaining that will require new mathematical advances

FUTURE WORK





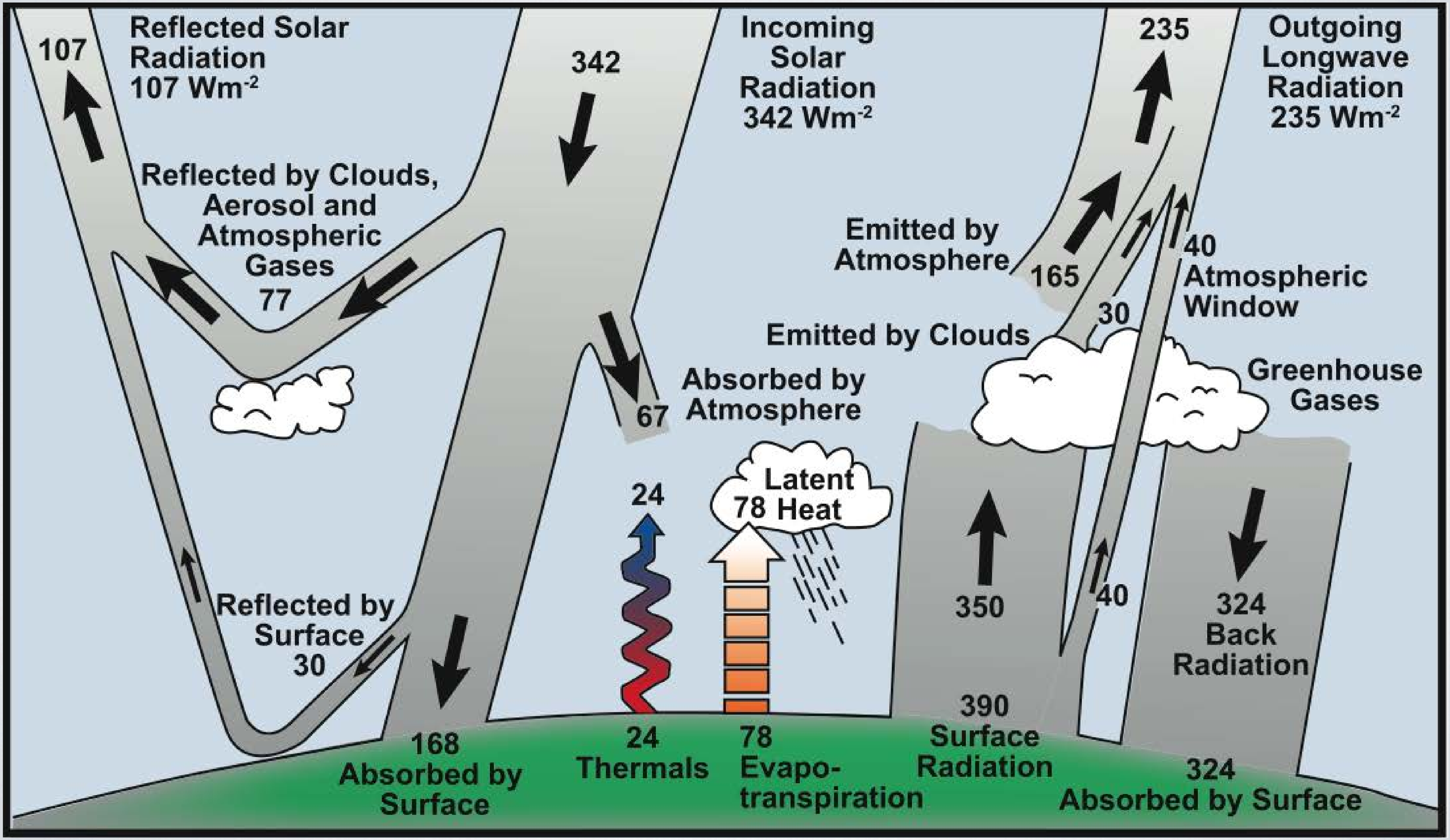
- Predict future climate scenarios
- Develop more efficient, environmentally friendly combustion processes
- Investigate other sources of renewable energy

THANK YOU !

EXTRA SLIDES

ATMOSPHERE ENERGY BALANCE

342 = 107 + 235



DENSITY FUNCTIONAL THEORY AND THE KOHN-SHAM EQUATIONS

$$
\begin{aligned}
E_{total}[\{\psi_i\}] &= \frac{1}{2}\sum_{i=1}^{n_e}\int_\Omega |\nabla\psi_i|^2 + \int_\Omega V_{ext}\rho \\
&+ \frac{1}{2}\int_\Omega \frac{\rho(r)\rho(r^{'})}{|r-r'|}drdr^{'} + E_{xc}(\rho),
\end{aligned}
$$

$$\rho = \sum_{i=1}^{n_e}|\psi_i(r)|^2,\ \int_\Omega \psi_i\psi_j = \delta_{i,j}$$

$$\left[-\frac{1}{2}\nabla^2 + V_{ext}(r) + \int \frac{\rho}{|r-r'|} + V_{xc}(\rho)\right]\psi_i = \epsilon_i\psi_i$$