Abstract

**Introduction**

**Climate change (**Causes, effects, history, societal challenges, numbers, IPCC reports**)**

***History***

In 1896 Svante Arrhenius published a paper, where the link between CO2 and the temperature of the ground is made for the first time (kilde til S. Arrh). In 1939 Guy Callendar argued, that anthropogenic emissions of CO2 had raised the CO2 content in the atmosphere by 10 percent since 1900 (kilde til Nasa artikel), while others (Roger Revelle) believed, that the biosphere would have absorbed the anthropogenic emissions. In the 1950s a group of oceanographers and geochemists were concerned with the CO2 concentration of the atmosphere because the ocean absorbs CO2, leading to more acidic surface water, which would affect sea life (kilde til Nasa artikel). In 1957 Charles David Keeling was hired at a postdoctoral scientist position by Roger Revelle and ordered to measure the CO2 concentration in the atmosphere at Mauna Loa, Hawaii. The CO2 concentration was measured with an infrared gas analyzer, that determines the absorption of an infrared light source through the surrounding atmosphere. Different atmospheric gasses absorb at different wavelengths, hence the adsorption at specific wavelengths can be related to atmospheric content of various gasses. (Basic, ingen kilde?)

The results of Keeling’s measurements were clear, the CO2 concentrations rose even during the short 18-month period of measurements. The measurements suggested that at most half of the anthropogenic CO2 emissions had been adsorbed by the biosphere. The plot showing CO2 concentration in parts per million as a function time was coined the Keeling curve and has been measured since, showing the increase in CO2 ppm rising from 313 ppm on march 29, 1958 to 421 ppm on august 2, 2023 (Kilde: Keeling Curve, ACS). Historical data on CO2 concentration in the atmosphere can be estimated before direct measurements were made via ice cores drilled up in Greenland and Antarctica. The past 800.000 years’ atmospheric content is trapped in the ice that froze each year and can be analyzed now, giving a long-term historical perspective and data used to model climate change (Kilde: Ice cores).

PLOT: Keeling curve?

***Causes***

The core mechanism behind climate change is based on the interaction between infrared and visible light and so called “Greenhouse gasses” (GHGs). Electromagnetic radiation from the sun enters the atmosphere and reaches earth’s surface, where some of it is adsorbed, heating the surface, and some is reflected, possibly leaving the atmosphere again. The heated surface in turn reradiates some of the energy as infrared radiation, as described by Planck’s radiation law. GHGs interact with the infrared radiation to adsorb and re-emit infrared radiation in all directions, about half back onto the earth’s surface. This mechanism allows energy from sunlight to pass through the earth’s atmosphere unobstructed by the GHGs, while returning half of the energy from reemitted infrared radiation from the surface, creating the “greenhouse effect” (Kilde: Greenhouse\_effect).

The carbon cycle consists of large amounts (gigatons) of CO2 being recycled through emitters like microbial respiration and decomposition and plant respiration and adsorbers, mainly photosynthesis. The anthropogenic carbon emissions ruin the balance of these REWRITE HERE

Without anthropogenic GHG emissions, there are still emissions from animals, that are absorbed by trees, plants, algae, etc. and

The majority

Note: Balance between earths CO2 emissions and absorbed. Carbon cycle. Burning fossil fuels containing hydrocarbons. Removal of wood

Note: Indsæt reaction hvor et fossil brændstof bliver brændt af f.eks. Butan. Og surprise, CO2 kommer ud.

***Effects***

Note: Direkte effekter: højere avg temp i luft og hav og sure have. Other effects: Is smelter, gletsjere smelter, sea levels are rising, Extreme weather events are increasing in frequency,

The direct effects of the anthropogenic GHG emissions are plentiful and a “threat to human wellbeing and health of the planet” (Kilde: IPCC feb 28). The average temperature of the atmosphere increases and has increased around 1.1 degrees Celsius since 1880 (Kilde: Earth observatory Nasa), projected to make 20 % of the planet a “barely livable” zone purely because of the heat (Kilde: IPCC). The oceans are getting warmer and more acidic, due to the ocean absorbing 20 to 30 percent of all anthropogenic CO2,emissions posing a threat to ecosystems that inhabit the oceans (Kilde: Earth obs Nasa). Ice sheets on Greenland and Antarctica have declined in mass, leading to increasing sea levels, that threaten to flood the homes of 300 million people (Kilde: New elevation data). Furthermore, the frequency of extreme weather events is increasing (Kilde: CSSR ’17).

From all this, it is apparent, that climate change is an issue on an apocalyptic scale, that has to be addressed in order to secure human wellbeing and existence on earth.

Note: Slut af med: og derfor har vi brug for et energisystem der kører på renewable energy sources, og det inkluderer både produktionen, lagring, etc.

Fuel Cells

Catalysis theory in general

Formic Acid Oxidation (Already close to CO2 in structure, compare to other species like methanol, ethanol. More effective with fever electron transfers and steps. Plot similar to the one from Jack with energy efficiencies)

Green fuels

Possible oxidation reactions (As Alexander showed in article)

Free energy diagrams

Modelling the activity of the two-step reaction

DFT machinery

High-Entropy Alloys (Hvorfor – tune poisoning effect) motivation

PEM fuel cell?

Overpotential?

Sabatiers Principle

**Methods**

Making data – show all Jack’s data and ref and my “own” data

Slabs for testing CO-OH slide reaction

Slabs for estimating H+COOH neighbor interactions

Slabs for estimating swim ring efficiency

Setting reference energies

Energy prediction models for adsorbate binding energies (With HEA and SWR data, hollow-site model, on-top model, mixed-site model) and all the equations and figures of them would be nice

Show a fcc(111) surface and hollow, on-top, mixed site

Using energy prediction models on simulated surfaces

Plotting them H vs COOH

Bayesian optimization of pair energies – searching for better composition

Coverage simulations and all the logic involved.

The random swim-ring mixture

**Conclusion**

Neighbor DFT data

Swim rings

Good composition found?

Method useful?

References

Notes about writing:

In Jack’s thesis he had these headlines between Introduction and Conclusion:

“Catalyst Discovery Using High-Entropy Alloys (?)

Calculating Adsorption Energies with Density Functional Theory (?)

Predicting DFT Adsorption Energies (?)

Optimizing the Composition (?)

Limitations of Methodology (?)”