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). Note: Ice cores gives CO2 ppm estimates.

Historical CO2 concentrations have been estimated from ice cores FORTSÆT HER (Kilde: Ice cores)

Note: Measuring temperature

***Causes***

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

Note: Greenhouse gasses (GHG)

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

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.

***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 greenhouse gas 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)

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 (?)”