Understanding Atmospheric Chemistry using Graph-Theory, Visualisation and Machine Learning.

Dan Ellis

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Veritatem inquirenti, semel in vita de omnibus, quantum fieri potest, esse dubitandu:
In order to seek truth, it is necessary once in the course of our life, to doubt, as far as possible, of all things.

- Descartes, Rene, *Principles of Philosophy*

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Chapter 1

Introduction

"In the beginning the Universe was created. This has made a lot of people very angry and been widely regarded as a bad move"

- Douglas Adams, *The Restaurant at the End of the Universe*

A Preface on Humanity and the Climate

The development of humanity is not unlike the chirography of an Aristotelian tragedy. It starts with a simple/primitive species cradling a noble cause - to improve their chances of survival. Here the protagonist (humankind) develops a fatal flaw: an insecurity and latent distruction of their home due to a sudden rise to power. Having acknowleged this flaw, we now strive to imporve our understanding of the universe, correct past mistakes and stem the tide of inevitable change.

With tragedy being an imitation not of humanity, but of action and life, happiness and misery, it is only expected that such a comparison to our current affairs should stir feelings of catharsis when exploring our need for research and scientific advancement. It is with that I begin this thesis with the begining of the planet, its atmosphere and consequently the beginning of humankind.

1.1 Whence

This section describes the intial formation of an atmosphere, how this led to life, and ultimately the human race.

1.1.1 Formation of the Atmosphere

4.5 billion years ago the Earth began as a disk of dust and gas orbiting our sun. As these gasses move about, resonant drag instability led to the clumping of dust particles, Hopkins and Squire [2018]; Woo [2018]. As these 'clumps' become denser, other forces come in to play, further increasing the size - eventually forming the hot mix of gas and solid which became the Earth.

In its cooling, the newly formed planet began to accumelate primodial gasses from the vollotile componenets of the gas cloud - forming an atmosphere. These gasess were then supplemented through outgassing (volcanic eruptions). At this point in time oxygen was not only absent in the atmopshere, but also had many siks within the Earths anoxidised crust. It was not until oxygenic photosynthesis (Peretó [2011]) that the concentrations of oxygen in the atmosphere started to increase. Eventually the development of multicellular cyanobacteria[1] resulted in biologically induced oxygen accumelating in the atmosphere, University of Zurich [2013]. This led to the most significant climate event in the planets history: the Great Oxigenation Event (2.5 billion years ago), Planavsky et al. [2014]. This increase of oxygen allowed oragnisms to become larger and more active, eventually resulting in the human race.

[1] The phylum of phtosynthetic prokaryotic (cells not containing a distinct nucleus) bacteria - e.g. blue-green algae

1.1.2 Rise of the Homo Spiens ('Wise Man')

About x million years ago there were many varieties of the homo genus. With the development of the human brain, energy transfer changed. A larger brain required more fuel, and therefore with the development of cooking[2] humans were able to increase their...

This led to the first know source of indoor air pollution.

Ever since we have experienced issues regarding to this...

As part of this air pollution and climate have always been a concern for the human race. Concerns about lead in the air can be documented back as far as 6000 years ago [se ref,], in ancient Rome [1145] and in 1285 where after a visit from Queen of England to a coal burning to Nottingham, the first air pollution act was deployed [1147].

air pollution = animals

air qulaity pollicy kingxx

With the this increased capability, a language capable of communicating information, allowing for the ability to not only hunt larger prey but also. Ability to metaphorical, allowed fruther knwoplege transfer , cvave paings and metaphoirical for people over 150 ....

REFERENCES TO OTHER CHAPTERS... - vis - accounting via metaphors - and an interest in science, and atmosphere

1.2 Motivation

1.3 composition of the atmosphere

Paper atmospere

main o2 and N , however billions each of these can be responsible for other reactions.

Mention OH mention O3 and pans Mention lifetimes.

[2] The first known case of indoor air pollution

1.4 Air Quality

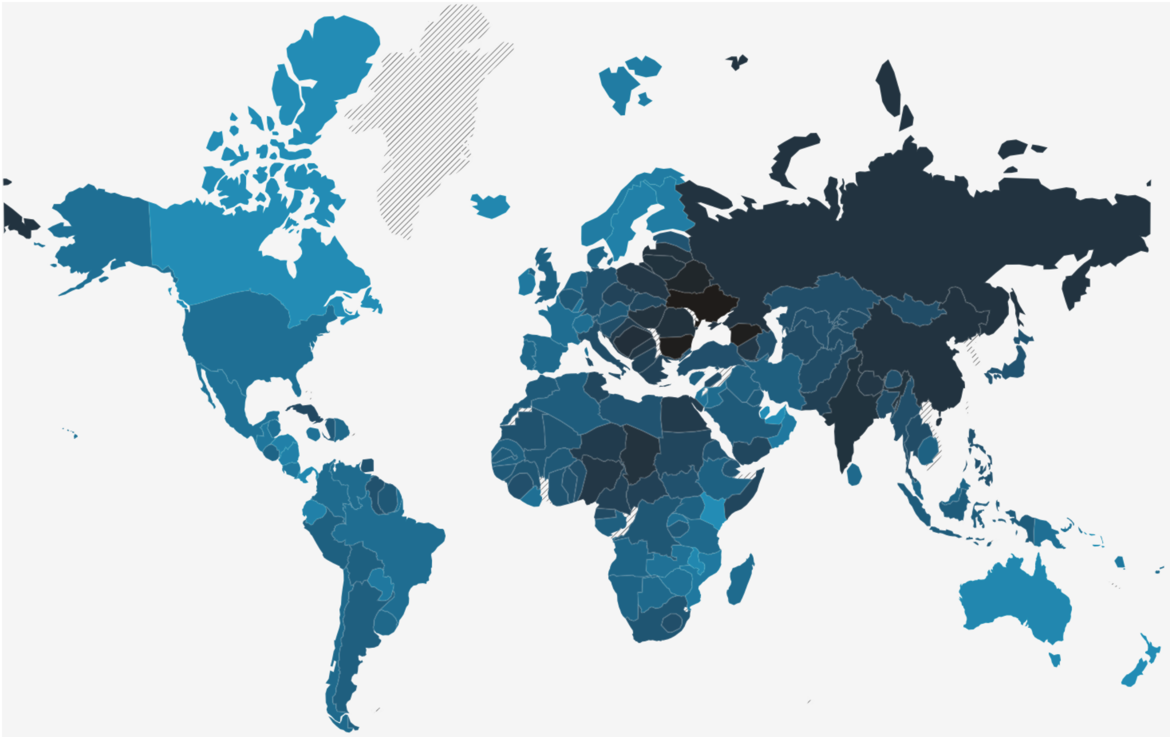

Figure 1.1: **Deaths attributed to air pollution REF WHO 16**

1.5 Changing Climate

The main removal

1.5.1 HOx Cycle

1.6 Ozone and its role

Ozone has two roles within the atmosphere. High up in the stratosphere it servers as a barrier to dangerous ultraviolet radiation. The importance of this was discovered in (HOLE PAPER) where the release of CloroFlouroCarbons from deodorants produced ...

However within the troposhere (<15k?) the production and loss of ozone has a direct impact on human life. Polluted environments, such as industrial London, SMOG, Clean air act.

1.7 The NOx cycle

Nitrogen Oxides (NOx) come predominantly from motor verhicles and power stations and can cause respiotory problems in children and asmatics [se1261]. They also play an important role in the formation and destruction of ozone.

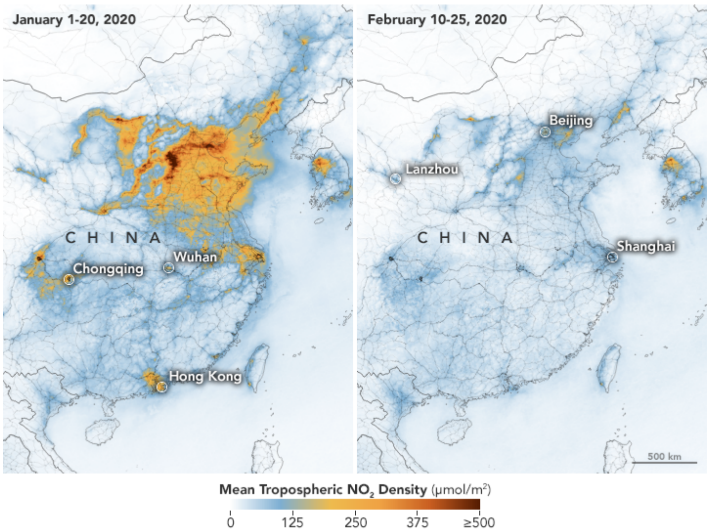

Figure 1.2: **Changes in NOx concentrations due to anthropogenic emissions.** A reduction in activity and trasport resutls in a large decrease of Nitrogen oxide concentrations in the troposphere. Source: Stevens [2020]

VOC

1.8 Modelling the Earth

In the previous section the air quality and its detrimental effects on human health was seen to influence polcicy for cities and industry. Koyoto, Islands suing powerstations.

For a policy to be passed there needs to not only evidence of the problem, but a strong suggestion that any proposed changes will have the desired effect. As it is not possible to perform experiments on complex, and often unknown, chemistry at every location on the planet, we are forced to rely on the numerical simulation of the Earth System, and the constituent parts within it.

1.8.1 Earth System Models (ESM)

ESMs are models capable of predict past or future interactions of the planetary system. They represnt our foremost understanding of the complex interplay between land-surface (geosphere), ocean (hydrosphere), ice (cryosphere) and the air (atmosphere), and act as a surrogate to manual experimentation

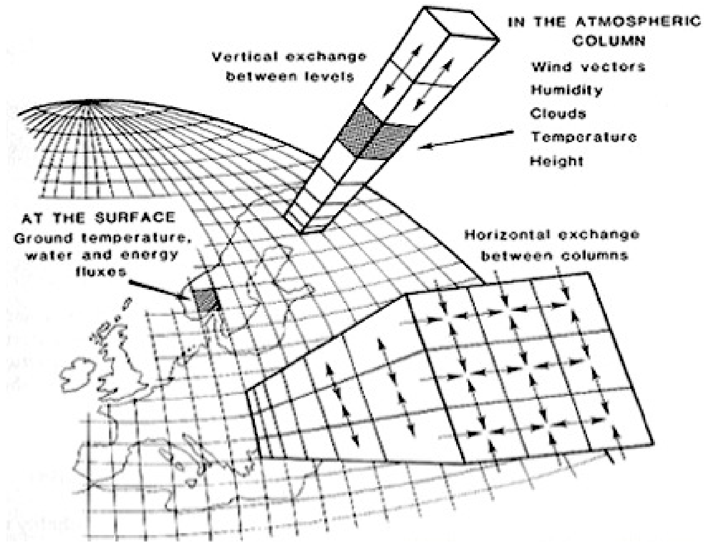

Figure 1.3: **A diagram showing the longitudal, lateral and vertical decomposition of a 3D global model.** Source: [Henderson-Sellers, 2015]

- which is just not possible on the global scale.

ESMs can be split into their individial parts. One example of this is the Chemistry section of the Goddard Earth Observing System (an integrated ESM and data assimulation model hosted by NASAs Goddard space flight centre [?]) - GEOS Chem. GEOS-Chem is a global 3D model of atmospheric chemistry which is driven by the meteorology provided by NASA [GEOS-Chem, 2020]. Here the earth is split up into cubic sphere cells longitudally and latitudally, as well as vertically (Figure 1.3)[3]. Each one of these cells performs several purtubations of the chemistry within them, before any long-lived species are transported, and the process is repeated. If extracted separately a single one of these cells may be used to explore the sensetivity of different species for a range of input conditions. This is the bases of the atmospheric box model.

1.8.2 The box model.

In exploring the sensetivities of individual species within a simulation, it is possible to use a zero dimensional box model. This is in essence a single cell within the global structure, constrained in location and height (pressure).

mechanism,

integrator,

etc.

[3]This image is not from GEOS-Chem.

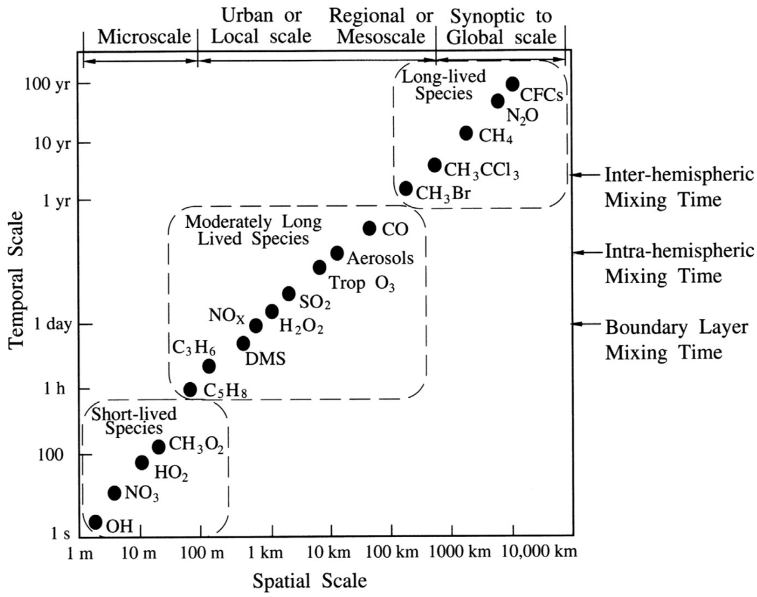

Figure 1.4: **Spatial and temporal scales of variability of atmospheric species.** Source: [Seinfeld and Pandis, 2016]

1.8.2.1 Chemical Mechanisms

Mechanisms are at the heart of every chemistry simulation. They are a mathematical representation of the possible reactions (and the rates at which these may occur) for every s

The atmosphere consists of thousands of species, with tens of thousands of reactions between them.

These models represent real wodlc reactions

In modelling these we can describe their rate of production and loss with respect to the species they react with.

1.8.3 Numerical integration

For example, it is possible to figure out how quickly each species in a reaction is changing if the reaction mechanism (the exact way it happe ns) and some simple data are known. This representation of how quickly the concentrations are changing is the same as a slope, or derivative. Integration allows us to find the actual change over time and not just how quickly the change is happening. Fo r example, given the following reaction,

In a mechanism we are concerned with calculating how quickly a species changes within the chemical system. Taking the reaction of N_2O_5 (Equation 1.1) we can write the rate of change for each species over time (Equation 1.2)[4]. In integrating this equation, we are able to calculate the actual change in

[4] This is also known as the flux.

concentration (Equation 1.3) - this is the foundation of atmospheric models.

$$N_2O_5 \longrightarrow NO_2 + NO_3 \tag{1.1}$$

$$d[N_2O_5]/dt \longrightarrow d[NO_2]/dt + d[NO_3]/dt \tag{1.2}$$

$$\int d[N_2O_5]/dt \longrightarrow \int d[NO_2]/dt + \int d[NO_3]/dt \tag{1.3}$$

1.8.3.1 Non-Stiff Equations

Computational systems cannot integrate numbers analytically we rely on a series of computational algorithms. Since integration is the calculation of the area under a curve, the simplest of these

1.8.3.2 Numerically stiff equations (atmospheric chemistry)

Figure 1.4 shows the lifetimes of species can range between x orders of magnitude, similarly the componenets for each reaction (differential equation) evolve on significantly different timescales. This makes the atmospheric chemical mecahnism

1.8.4 The model development cycle

Scientific understanding is the product of many cycles of trial and error, Figure 1.5. In atmospheric chemistry we start with a hypothesis or a question, e.g. will changing X have a negative response on Y. We then construct a theoretical model to represent the chemsistry within. This chemistry is updated to reflect the rates and reactions that have been recorded in laboratory/chamber experiments. This cycle is then repeated until the model and real-world observations produce a comparable result.

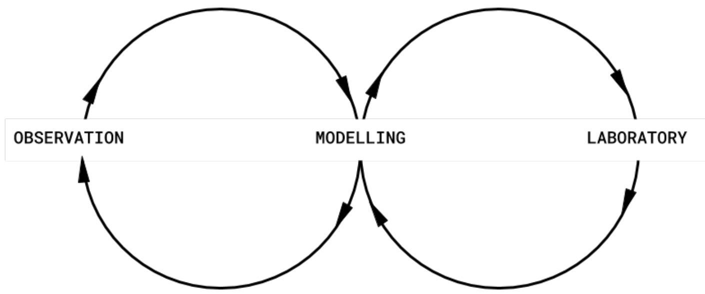

Figure 1.5: **The scientific development cycle.**This shows the iterative nature between modelling, observation and laboratory experimentation

ESM

A series of box models.

1.8.5 The Dynamically Simple Model of Atmospheric Chemical Complexity

1.9 Thesis Layout

This thesis will explore a series of methods for describing and understaning the complex chemistry which may exist as part of an atmospheric chemistry mechanism. The mechanism used is a near-explicit representation of our foremost understanding of how gas phase chemistry in the troposphere reacts - the Master Chemical Mechanism, [?].

We begin by exploring the use of visualisation to convey complex scientific data (**??**). Next we apply this to the representation of species in a mechanism, and the relationships between them. To do this it is found that the node-link style graph format is the most beneficial, the use of which is then explored further (**??**). **??**

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