

Atmospheric Modelling Keeping an Eye on Weather, Climate & Pollution

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Atmospheric modelling is a complex affair involving an intricate synchronisation of Physics, Chemistry & Computers to forecast weather, climate & air pollution.

CHECKING weather forecasts has become embedded in our day-to-day life today. We check the day's temperature. We check whether it's going to rain in the coming days to plan for important events. We also check the weather forecasts to plan our holidays and trips. Today, with worsening air pollution, we even check for predictions about air quality.

Air pollution has been occurring naturally ever since the formation of the Earth. But it was during the industrialisation era in the 18th century when it started increasing dramatically. However, back then air pollution was considered more of a regulatory issue and not science.

This changed when several severe air pollution episodes in the 20th century were found to be caused by complex atmospheric chemistry and changes in weather conditions. The so-called great smog of London (1952) was caused by low-wind atmospheric conditions of winter which were trapping the emissions from coal-burning and industries. In sharp contrast, the smog in Los Angeles in the 1940s was a result of photochemical ozone production through reactions of hydrocarbons and nitrogen oxides catalysed by intense sunlight during the summers.

These along with several other major pollution episodes established that air pollution is governed by a combination of physical and complex chemical processes. This was the time when air pollution studies and weather science (meteorology)

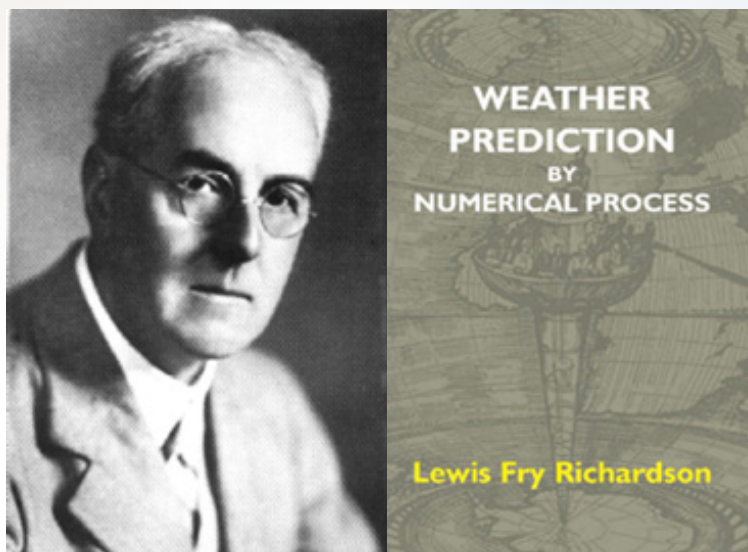
were merging. The large health impacts including deaths during pollution episodes highlighted the need for science-informed policies for controlling air pollution. Accurate modelling of air pollution started gaining more and more attention. However, atmospheric modelling is extremely complex and requires an understanding of several parameters.

Atmosphere + Emissions – A Deadly Cocktail

Combinations of atmospheric conditions and emissions cause recurring and widespread air pollution typically every year in both winters and summers, most notably in the Indo-Gangetic Plain (IGP) and Northern China Plain (NCP).

Research has revealed that health risks are the most pronounced due to fine Particulate Matter (PM_{2.5}) i.e., aerosol particles smaller than 2.5 μm in diameter. In addition, Ozone (O₃), Carbon Monoxide (CO), Nitrogen Oxides (NO_x), Sulfur Dioxide (SO₂), Volatile Organic Compounds (VOCs),

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Lewis Fry Richardson

Supercomputing

Atmospheric modelling relies greatly on the high-performance computing resources supported by supercomputers. Supercomputers allow calculation of over thousands of processors parallelly. A software called the Modular Earth Submodel System (MESSy) has been developed to provide a framework for combining Earth System Models with flexible complexity. The developers received the Heinz Billing Award for the Advancement of Scientific Computation in 2005.

With increasing knowledge resulting in more complex models, more powerful computers are being developed. Building up and maintaining such resources is a huge task and therefore, many users and organisations have started opting for the on-demand resources in pay-as-you-go mode through cloud computing. The need for more powerful computers and progress in scientific understanding and, therefore, in the models is continuous. The world's most powerful supercomputers are in the US, Europe, China and Japan.

The National Supercomputing Mission (NSM), an initiative of the Government of India announced in 2015, aims to boost indigenous efforts toward supercomputing capabilities in the nation to boost research and developments. As of June 2021, three Indian supercomputers were ranked among the world's top 500 supercomputers - *PARAM Siddhi-AI* in the Center for Development of Advanced Computing; *Pratyush* at the Indian Institute of Tropical Meteorology, and *Mihir* at the National Centre for Medium-Range Weather Forecasting.

More recently in 2022, *Param Pravega* with a total supercomputing capacity of 3.3 petaflops, one of the most powerful supercomputers in the country, was installed at the Indian Institute of Science in Bengaluru under the NSM. With several supercomputers coming up under NSM, India is evolving fast to join the ranks of frontrunners on the global map. Installation of supercomputers at premier institutions in India will substantially enhance the capability to pursue earth system modelling, besides other frontline research and applications.



Shivay is a supercomputer assembled by C-DAC India in the series of PARAM Supercomputers

etc. also contribute to the degradation of air quality. As per the World Health Organization (WHO), almost all the population of the globe breathes air exceeding the air quality standards.

It is important to note that air pollution has adverse impacts not only on human health but also on crop productivity and therefore directly on the economy. There are vital links of air quality with clouds and rainfall, Earth's radiation budget and thus with the changing climate. Although quantitative understanding of such links is still developing, it has become clear that the understanding of air pollution over local to global scales and its impact on health and climate is of paramount significance for both science and society.

Modelling — Interplay of Physics, Chemistry & Computers

The natural and man-made processes governing air pollution are remarkably diverse and play their roles over different horizontal scales. The daily and seasonal changes in emissions from traffic, industries, fires in forests and agricultural fields, and natural variability in weather highly complicate

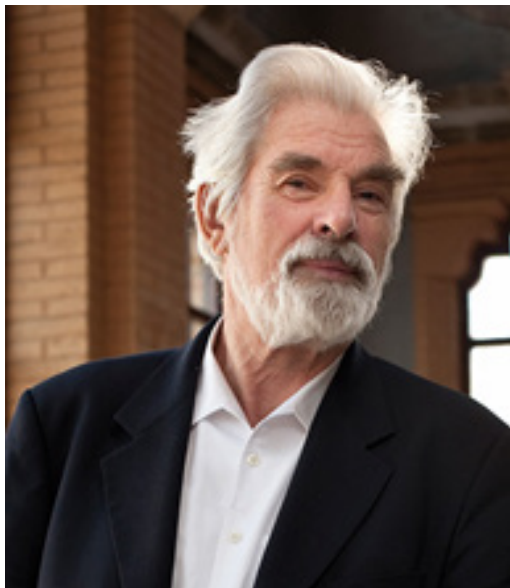
the nature of pollution over a region. To comprehend this, scientists compile and condense all the knowledge of physics and chemistry of the Earth's atmosphere in the form of computer programs, called "models". These atmospheric models use well-known equations of physics, such as the continuity equation, Newton's second law of motion, and thermodynamics.

An interesting story is that it was Lewis Fry Richardson, an ambulance driver for the French army during World War I, who worked in his free time and developed the first numerical weather model. He solved simplified equations by performing integration by hand. He did not get satisfactory results but was successful in coming up with a methodology which he described in a landmark book *Weather Prediction by Numerical Process* published in 1922. Since there were no means to carry out extensive computations at that time, further work in this direction could not be done. The first major breakthrough came when the world's first digital computer — ENIAC — was built and weather modelling was proposed to be its main application.

The version of the atmospheric model developed by John von Neumann and Jule Charney in the early 1950s captured features of large-scale atmospheric flows successfully. Scientists started taking a particularly keen interest in the chemistry of the Earth's atmosphere after discovering severe depletion of the ozone layer in the stratosphere — more familiarly known today as the ozone hole. Chapman was successful in simulating the peak of ozone and in explaining important aspects of its chemistry.

Paul Crutzen made pioneering contributions in unravelling the role of nitrogen oxides in the loss of stratospheric ozone. In fact, the cancellation of the plans for Supersonic aircrafts was in view of these findings. Later Mario Molina and Sherwood Rowland identified the roles of chlorofluorocarbon gases also. The trio, Crutzen, Molina and Sherwood were awarded the Nobel prize in Chemistry in 1995 for these pioneering works on the ozone layer.

With the availability of more powerful computers, the development of climate models or the General Circulation



Manabe and Hasselmann: Nobel Prize
Winners of Physics (2021)

Recent Studies

Global model results have helped immensely in filling the gaps of observations over regions with sparse monitoring of air quality. A key result from global modelling studies (<https://www.nature.com/articles/nature15371>) shows that air pollution, in particular the fine Particulate Matter (PM_{2.5}) can lead to more than 3 million premature deaths globally every year. The researchers also noticed diversity in the major sources over India than those in the USA and Europe. Simulation considering business-as-usual scenarios predicts that the health impacts of pollution may be doubled by 2050.



Picture Courtesy: Jimmy Nuetron (CCA-SA 4.0)

Another study based on a regional model revealed that ozone pollution in India substantially reduces the agricultural productivity of wheat by about 20% and rice by 6%. The economic losses due to the reduction in crop productivity are suggested to increase due to an increase in the crop prices and that controlling air pollution will be even more important.



Photo Credit: Cameron Strandberg (CCA-SA 2.0)

Models (GCM) began. In this direction, very notable contributions were made by Norman Phillips, Joseph Smagorinsky, Syukuro Manabe, Yale Mintz, Akio Arakawa, Warren Washington and Akira Kasahara.

Syukuro Manabe led the development of the climate model in the 1960s and subsequent model developments by Klaus Hasselmann established the abilities of models to make predictions of weather as well as climate. Their works unravelled that increase in atmospheric carbon dioxide due to human activities was leading to global warming. These works laid the foundation for the development of climate models being applied today. Since then, continuous model developments and applications are going on.

New observations from state-of-the-art instruments, satellite data, and laboratory experiments helped in better understanding of atmospheric processes and thus in improving the models. Manabe and Hasselmann were awarded the Noble Prize in Physics in 2021, along with Giorgio Parisi for their outstanding contributions to the modelling of complex systems.

Three-dimensional air quality modelling started in 1960-1970 and the global scale models came into existence in the 1980s with important contributions from Hiram Levy, Michael Prathar, and Peter Zimmermann. These “air quality” or “photochemical” models include additional details on a variety of emission sources and chemistry of different gases and particulate matter (also called aerosols), besides

Applications of Artificial Intelligence/Machine Learning

Machine learning/artificial intelligence has emerged as another very powerful modelling technique in recent years. Unlike the conventional models based on knowledge of physics and chemistry, the machine learning technique utilises data for building the models. Studies have revealed a strong potential of machine learning for simulating the air quality variations including over the highly complex Himalayan foothills region (<https://www.nature.com/articles/s41598-021-01824-z>). These techniques are being further explored to be combined with conventional models for parameterising highly complex processes.

The main advantages of this technique are that the less understood processes can also be simulated with high skill and machine learning codes are computationally less expensive than the conventional atmospheric models.

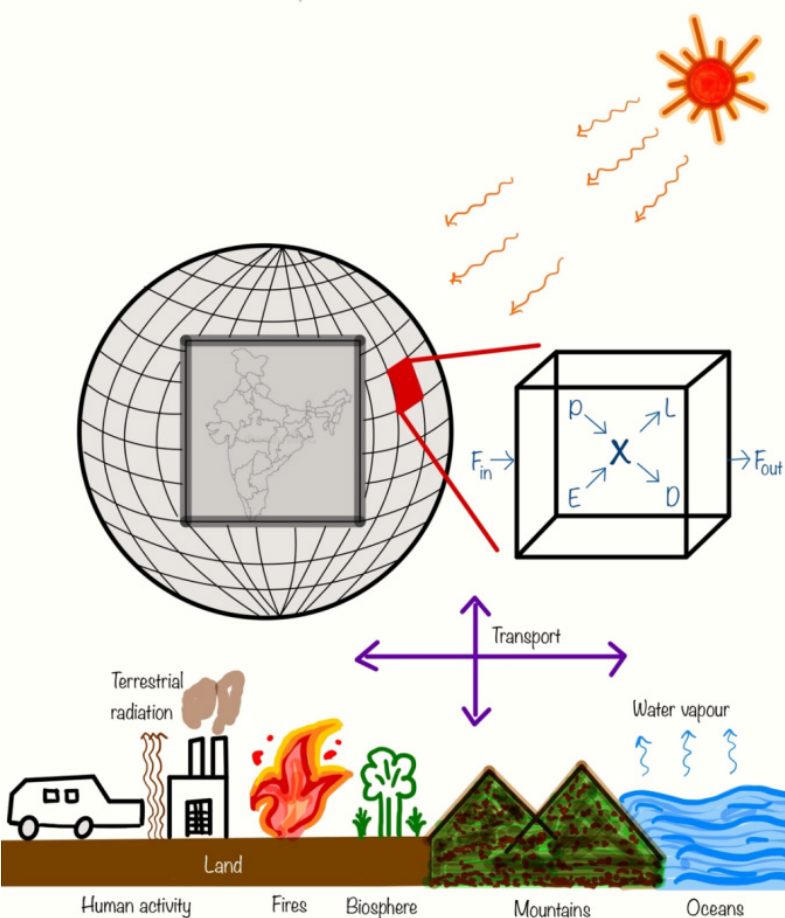


Figure 1: A simplified cartoon of important processes affecting air quality. Models divide the region of interest into boxes or grid cells and numerically compute the sources (F_{in} , P , E) and sinks (F_{out} , L , D) of pollutants (here called X).

information on atmospheric conditions as in weather models. Due to a large number of processes occurring simultaneously and involved complexities, atmospheric models are highly complex and require supercomputers to do the simulations. Models showing good agreements with observations are utilised to solve problems of scientific as well as wider public interests.

Suite of Models

A suite of models applicable over different horizontal scales — global, regional, and local-scale — are being used globally. The global models simulate the air quality over the entire globe although the spatial resolution is coarse. Whereas the regional-scale models focus over a particular region to make high-resolution simulations but they rely on results from global models to account for the long-range or inter-continental transport.

Typically, all atmospheric models intend to account for the effects of emissions from various natural and man-made sources, variations in the atmospheric conditions often called meteorology, and the role of transport to compute air quality changes. Figure 1 depicts the key processes in the Earth's atmosphere.

It is clear from this figure that the processes controlling air quality over the region of interest can be remarkably diverse. Urbanisation, industrialisation, and traffic have enhanced the burning of fossil fuels in an unprecedented manner. Besides the natural biogenic emissions, forest fires and the burning

of crop residues in agricultural fields are also shown to have profound impacts.

The globe or a particular region is divided into boxes, called the grid cells (Figure 1) and then sources and sinks of pollutants (suppose X) are computed. Major production terms may include chemical production (P), transport from upwind regions (F_{in}), and direct emission (E). The major sinks include chemical loss (L), transport out from the cell (F_{out}) and deposition (D) to the surface. Effects of many processes such as convection, boundary layer, radiation, etc. are included through parameterisation schemes.

To make such computations, atmospheric modelling requires high-performance computing clusters or supercomputers. An exception is the local-scale models e.g., photochemical box, radiative transfer, etc., which can be run on desktops or laptops since these models do computations for a single air parcel or a vertical column.

These models have proved valuable as they directly allow incorporating observations so the effects of uncertainties in emissions and meteorological simulations can be minimal. The major advantage is that local box models can treat air chemistry with all details, i.e., about 2000 chemical species participating in 5000 different reactions, without the need for any simplifications as in the case of global and regional models. If the whole globe is considered a single box, then F_{in} and F_{out} terms will vanish.

Simulations vs Real-time Observations

Before applications to problems of scientific and societal interests, the model simulations are evaluated against real-world observations. The observations of atmospheric composition and meteorological conditions are being conducted from numerous platforms such as the ground-based monitoring stations, balloon-borne sensors, instruments aboard satellites in space, and aircraft-based campaigns.

Models perform differently over different regions of the globe and therefore to evaluate and improve the models, global efforts are essential. The unprecedented lockdowns implemented to stop the spread of the novel Coronavirus (COVID-19) resulted in substantial shutting down of human activities, traffic, and industries in different regions of the world including India. The observed changes in air quality during these circumstances offered scientists a rare and unique opportunity to test the effects of human activities on air pollution. The studies also revealed the importance of meteorological variations, natural dust emissions, and non-linearities in air chemistry in controlling air quality during the near-background conditions of the lockdown.

Local-scale models have offered the opportunity to incorporate direct measurements to have more certain predictions. The radiative transfer models have helped in making accurate estimations of the climatic effects of particulate matter. Photochemical box models have allowed us to exploit available measurements to predict the concentrations of radicals (<https://www.sciencedirect.com/science/article/abs/pii/S004565352200563X>) that control the atmosphere's self-cleaning capacity but are extremely difficult to directly measure.

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Despite huge progress in air quality modelling since its inception, the models still have substantial uncertainties owing to uncertain emission inputs and biases in meteorological simulations. Parameterisations of physical processes developed for one part of the world may not be readily applicable in another part with very different climatic conditions. Simplified treatments of air chemistry in the regional and global models are another source of uncertainty. These models fail to adequately resolve highly complex geographical terrains such as the Himalayas in the north of the Indian subcontinent.

With the availability of more intense computational resources, now model simulations are also being done at 1 km x 1 km resolutions and chemistry of more species are being included to overcome these challenges. Assimilation of observations into models has improved the predictions very much and currently real-time ground- and satellite-based observations are infused in models which have significantly improved the forecasts. Besides providing early warning for the residents and governments to take necessary steps, models are helping to identify the major sources of pollution in near real-time (<https://www.nature.com/articles/d41586-022-00332-y>).

Besides the long-term climate simulations, emphasis is also being given to the so-called chemical climate which can tell us how the air composition will evolve in the long-term future depending upon the choices that we make in terms of anthropogenic emissions (<https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2021AV000399>) and through feedbacks of global warming.

While the data assimilations are helping to improve the predictions over short-term timescales, continuous basic research in better understanding the physics and chemistry of Earth's atmosphere to achieve accurate simulations of future air quality and climate are imperative.

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