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Mark Z. Jacobson
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Fundamentals of Atmospheric Modeling

This comprehensive text describes the atmospheric processes, numerical methods, and computational techniques required for a scientist to successfully study air pollution and meteorology.

Computer modeling has become a powerful tool in modern atmospheric sciences, combining the disciplines of meteorology, physics, mathematics, chemistry, computer sciences, and, to a lesser extent, geology, biology, microbiology, and oceanographic sciences. This text presents fundamental equations that describe physical, chemical, and dynamical processes in the atmosphere, and it provides numerical methods to solve these equations. Along with classic methods of simulating dynamical meteorology, the text contains several numerical techniques for simulating gas and aerosol processes not available in any other text.

The book has been developed from the author's graduate courses and research at Stanford University and contains homework and computer programming assignments. It is a valuable textbook for graduate and upper-level undergraduate courses in atmospheric sciences and meteorology. It will also be useful for courses in earth sciences, environmental sciences, and applied mathematics.

Mark Z. Jacobson is currently Professor of Civil and Environmental Engineering at Stanford University. He received a B.S. with distinction in Civil Engineering, a B.A. with distinction in Economics, an M.S. in Environmental Engineering from Stanford University in 1988, and an M.S. and PhD in Atmospheric Sciences from UCLA in 1991 and 1994, respectively. In addition to numerous awards and scholarships, he received an NCAA-ITCA scholar-athlete of the year award while at Stanford University, in 1985, 1986, and 1987.

To Dionna and Daniel

Fundamentals of Atmospheric Modeling

MARK Z. JACOBSON

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http://efml.stanford.edu/FAMbook/FAMbook.html

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Preface

Modern atmospheric science is a field that combines meteorology, physics, mathematics, chemistry, computer sciences, and to a lesser extent geology, biology, microbiology, and oceanographic sciences. Until the late 1940s scientific studies of the atmosphere were limited primarily to studies of the weather. At that time, heightened concern about air pollution caused a surge of atmospheric chemistry studies, and computer modeling of meteorology and air pollution commenced. Since the late 1940s, the number of meteorological and air-pollution studies has increased rapidly, and meteorological and air-pollution models have slowly merged.

BRIEF HISTORY OF METEOROLOGICAL SCIENCES

The history of atmospheric sciences begins with weather forecasting. Forecasting originally grew out of three needs – for farmers to produce crops, sailors to survive at sea, and populations to avoid weather-related disasters such as floods. Every society has forecast wind, rain, and other weather events. Some forecasts are embodied in platitudes and lore. Virgil stated, "Rain and wind increase after a thunderclap." The Zuni Indians had a saying, "If the first thunder is from the east, winter is over." Human experiences with the weather have led to more recent forecast rhymes, such as, "Rainbow in morning, sailors take warning. Rainbow at night, a sailor's delight."

Primitive forecasts have also been made based on animal and insect behavior or the presence of a human ailment. Bird migration was thought to predict oncoming winds. This correlation has since proved unreliable. Rheumatism, arthritis, and gout have been associated with the onset of rain, but such ailments are usually unrelated to the weather. The presence of locusts has correctly been associated with rainfall in that locusts fly downwind until they reach an area of converging winds, where rain is likely to occur.

In the 1870s, forecasting based on observations and experience became a profession. Many felt that early professional forecasting was more of an art than a science, since it was not based on scientific theory. Although the number of data available to forecasters was large and increasing, the data were not always used. Data were gathered by observers who used instruments that measured winds, pressure, temperature, humidity, and rainfall. Many of these instruments had been developed over the previous two centuries, although ideas and crude technologies existed prior to that time.

Preface

The Greeks, around 430 B.C., may have been the first to measure winds. Yet, reliable instruments to measure wind force and direction were not developed until the seventeenth century. In 1667 Robert Hooke developed the **pressure-plate anemometer**, which measured the deflection and force of wind on a sheet of metal hanging vertically. This principle was used again in the **pressure-tube anemometer**, thought of earlier but not built until the 1740s. Windmills were used as early as 644 A.D. in Persia, but the first **cup anemometer**, which applies the principle of the windmill to measure wind speed, was not developed until the seventeenth century, in France. In the nineteenth century, additional work on the anemometer was carried out by T. R. Robinson and W. H. Dines.

The **mercury barometer**, used to measure air pressure, was invented in 1643 by Evangelista Torricelli (1608–1647), an associate of Galileo Galilei (1564–1642). Toricelli invented the barometer (*Encyclopedia Britannia* 1980)

> to make an instrument which might show the changes of the air, now heavier and coarser, now lighter and more subtle.

By 1663, the Royal Society of London had built its own barometer based on Torricelli's model. The **aneroid barometer**, which represented an advance over the mercury barometer, was not adequately developed until 1843. The aneroid barometer contains no fluid. Instead, it measures pressure by gauging the expansion and contraction of a tightly sealed metal cell that contains no air.

A third important invention for meteorologists was the thermometer. Prior to 1600, Galileo devised the **thermoscope**, which measured the expansion of air to estimate temperature changes. The instrument did not have a scale and was unreliable. Torricelli's mercury barometer, which contained fluid, led to the invention of the **liquid-in-glass thermometer** in Florence by the mid–seventeenth century. In the early eighteenth century, useful thermometer scales were developed by Gabriel Daniel Fahrenheit of Germany (1686–1736) and Anders Celsius of Sweden (1701–1744).

A fourth important invention was the **hygrometer**, which measures humidity. Leonardo da Vinci (1452–1519) was probably the first to implement a hygrometer. He based his idea on notes of Nicolas Cryfts, who suggested in 1450 that a hygroscope could be constructed with dried wool placed on a scale. The change in weight of the wool would give a rough idea of the change in humidity. Wood and seaweed were used later in place of wool. In the seventeenth century, gut, string, cord, and hair were also used to measure humidity, since the change in length of these materials with humidity could be measured crudely. The hair hygrometer is still used today, although another instrument, the **psychrometer**, is more accurate. A psychrometer consists of two liquid-in-glass thermometers mounted together, one with a dry bulb and the other with a bulb covered with a moistened cloth.

Following the inventions above, observations of pressure, temperature, humidity, wind force, wind direction, and rainfall became regular. By the nineteenth century, weather-station networks and meteorological tables were common. Observers gathered data and forecasters used the data to predict the weather, but neither observers nor forecasters applied significant theory in their work. Theoreticians studied physical laws of nature but did not take advantage of the abundance of data available.

One of the first weather theoreticians was Aristotle, who wrote *Meteorologica* about 340 B.C. In that text, Aristotle attempted to explain the cause of winds, clouds, rain, mist, dew, frost, snow, hail, thunder, lightning, thunderstorms, halos, rainbows, and mock suns. On the subject of winds, he wrote (Lee 1951)

> These, then are the most important different winds and their positions. There are two reasons for there being more winds from the northerly than from the southerly regions. First, our inhabited region lies towards the north; second, far more rain and snow is pushed up into this region because the other lies beneath the sun and its course. These melt and are absorbed by the earth and when subsequently heated by the sun and the earth's own heat cause a greater and more extensive exhalation.

On the subject of thunder, he wrote,

> Let us now explain lightning and thunder, and then whirlwinds, firewinds and thunderbolts: for the cause of all of them must be assumed to be the same. As we have said, there are two kinds of exhalation, moist and dry; and their combination (air) contains both potentially. It condenses into cloud, as we have explained before, and the condensation of clouds is thicker towards their farther limit. Heat when radiated disperses into the upper region. But any of the dry exhalation that gets trapped when the air is in process of cooling is forcibly ejected as the clouds condense and in its course strikes the surrounding clouds, and the noise caused by the impact is what we call thunder.

Aristotle's monograph established a method of qualitatively explaining meteorological problems. Since Aristotle was incorrect about nearly all his meteorological conclusions, *Meteorologica* was never regarded as a significant work. Aristotle made observations, as evidenced by diagrams and descriptions in *Meteorologica*, but he did not conduct experiments. Lacking experiments, his conclusions, while rational, were not scientifically based.

Aristotle's method of rationalizing observations with little or no experiment governed meteorological theory through the seventeenth century. In 1637, René Descartes (1596–1650) wrote *Les Météores*, a series of essays attached to *Discours de la Méthode*. In some parts of this work, Descartes improved upon Aristotle's treatise by discussing experiments. In other parts, Descartes merely expanded or reformulated many of Aristotle's explanations. On the subject of northerly winds, Descartes wrote (Olscamp 1965)

> We also observe that the north winds blow primarily during the day, that they come from above to below, and that they are very violent, cold and dry. You can see the explanation of this by considering that the earth EBFD [referring to a diagram] is covered with many clouds and mists near the poles E and F, where it is hardly heated by the sun at all; and that at B, where the sun is immediately overhead, it excites a

> quantity of vapors which are quite agitated by the action of its light and rise into the air very quickly, until they have risen so high that the resistance of their weight makes it easier for them to swerve, ...

Like Aristotle, Descartes was incorrect about many explanations. Despite some of the weaknesses of his work, Descartes is credited for being one of the first in meteorological sciences to form hypotheses and then to conduct experiments.

Between the seventeenth and mid–nineteenth centuries, knowledge of basic physics increased, but mathematics and physics were still not used rigorously to explain atmospheric behavior. In 1860, William Ferrel published a collection of papers that were the first to apply mathematical theory to fluid motions on a rotating earth. This work was the impetus behind the modern-day field of **dynamical meteorology**, which uses physics and mathematics to explain atmospheric motion.

Between 1860 and the early 1900s weather forecasting and theory advanced along separate paths. In 1903, Vilhelm Bjerknes of Norway (1862–1951) promulgated the idea that weather forecasting should be based on the laws of physics. This idea was not new, but Bjerknes advanced it further than others (Nebeker 1995). Bjerknes thought that weather could be described by seven primary variables – pressure, temperature, air density, air water content, and the three components of wind velocity. He also realized that many of the equations describing the change in these variables were physical laws already discovered. Such laws included the continuity equation for air, Newton's law of motion, the ideal-gas law, the hydrostatic equation, and the thermodynamic energy equation.

Bjerknes did not believe that prognostic meteorological equations could be solved analytically. He advocated the use of physical principles to operate on graphical observations to forecast the weather. This technique was called **graphical calculus**. Between 1913 and 1919, Lewis Fry Richardson (1881–1953), developed a different method of analyzing the equations describing the weather (Richardson 1922). The method involved simplifying the equations before solving them numerically by hand. Richardson was not satisfied, because data available to test his method were sparse, and predictions from his method were not accurate. Nevertheless, his was the first attempt to numerically predict the weather in detail (ibid.).

Until the 1940s, much of Richardson's work was ignored because of the lack of a means to carry out the large number of calculations required to implement his method. In 1946, John von Neumann (1903–1957), who was associated with work to build the first electronic computer, proposed a project to make weather forecasting its main application. The project was approved, and the first computer model of the atmosphere was planned. Among the workers on von Neumann's project was Jule Charney, who became director of the project in 1948. Charney made the first numerical forecast on the computer, ENIAC, with a one-dimensional model. Since that time, numerical models of weather prediction have become more elaborate, and computers have become faster.

Preface

BRIEF HISTORY OF AIR-POLLUTION SCIENCES

Meteorological science is an old and established field; air-pollution science has a shorter history. Natural air pollution has occurred on earth since the planet's formation. Fires, volcanic eruptions, meteorite impacts, and high winds all cause natural air-pollution. Human-made air-pollution problems have existed on urban scales for centuries and have resulted from burning of wood, vegetation, coal, oil, natural gas, waste, and chemicals.

Before the twentieth century, air pollution was not treated as a science but as a regulatory problem (Boubel et al. 1994). In Great Britain, emissions from furnaces and steam engines led to the Public Health Act of 1848. Emissions of hydrogen chloride from soap making led to the Alkali Act of 1863. In both cases, pollution abatement was controlled by agencies. In the nineteenth century, pollution abatement in the United States was delegated to municipalities. Regulations did not reduce pollution much, but they led to pollution control technologies, such as the scrubber for removing effluent gases from smokestacks and, later, the electrostatic precipitator for reducing particulate emissions from them.

Inventions unrelated to air-pollution regulation reduced some pollution problems. In the early twentieth century, the advent of the electric motor centralized sources of combustion at electric utilities, reducing local air pollution caused by the steam engine.

At the same time, widespread use of automobiles and other combustion processes increased pollution, especially in urban regions. Most noticeable was a layer of pollution that formed almost daily in Los Angeles, California. This pollution became so serious that an Air Pollution Control District was formed in Los Angeles in 1947. In 1949, the first National Air Pollution Symposium was held in Los Angeles. In 1951, Arie Haagen-Smit produced ozone in a laboratory from oxides of nitrogen and reactive organic gases, in the presence of solar radiation, and he suggested that these gases were the main constituents of Los Angeles air pollution. Such pollution became known as **photochemical smog**. Photochemical smog, due primarily to automobile emissions, has since been observed in most cities of the world.

The term **smog** was first coined in 1905 by Harold Antoine Des Voeux, who described the combination of smoke and fog he observed in cities in Great Britain. The smoke was due to chimney and stack emissions of coal combustion products. In December 1952, such smog resulted in over 4000 deaths in London. This fatal episode was not the first in London. Pollution resulting from coal combustion in the presence of fog is commonly referred to as **London-type smog.**

THE MERGING OF AIR-POLLUTION AND METEOROLOGICAL SCIENCES

In the 1950s, laboratory work was undertaken to better understand the formation of photochemical and London-type smog. Since the computer was already available, box models simulating atmospheric chemical reactions were immediately implemented. Between the 1950s and 1970s, air-pollution models, termed **air-quality models**, were expanded to three dimensions. Such models included treatment of transport, deposition, emissions, and gas chemistry. Most of these models used observed meteorological data as inputs. More recently, air quality models have used meteorological fields, either precalculated or calculated in real time, as inputs.

In the 1970s, atmospheric pollution problems, aside from urban air pollution, were increasingly recognized. Such problems included regional acid deposition, global ozone reduction, Antarctic ozone depletion, and global climate change. Initially, ozone depletion and climate change problems were treated separately by dynamical meteorologists and atmospheric chemists. More recently, computer models that incorporate atmospheric chemistry and dynamical meteorology have been used to study these problems.

The purposes of this book are to provide (1) a physical understanding of dynamical meteorology, gas chemistry, aerosol microphysics and chemistry, radiation, and cloud processes in the atmosphere, (2) a description of numerical methods and computational techniques used to simulate these processes, and (3) a catalog of steps required to construct, apply, and test a numerical model.

After the overview in the first chapter, atmospheric structure, composition, and thermodynamics are described in Chapter 2. In Chapters 3–5, basic equations describing dynamical meteorology are derived. In Chapter 6, numerical methods of solving partial differential equations are discussed. A finite-difference technique of solving dynamical meteorological equations is provided in Chapter 7. In Chapters 8 and 9, boundary-layer and cloud processes, respectively, are described. Chapter 10 introduces radiation. Chapters 11–13 focus on photochemistry and numerical methods of solving chemical equations. Chapters 14–19 describe aerosol physical and chemical processes. Chapter 20 describes sedimentation and dry deposition. Chapter 21 outlines computer model development, application, and testing.

The book is designed as a graduate, upper-level undergraduate, and research text. The text assumes students have a basic physical science, mathematical, and computational background. Both Système Internationale (SI) and centimeter-gram-second (CGS) units are used. Dynamical meteorologists often use SI units, and atmospheric chemists often use CGS units. Some chemical variables, such as gas concentrations, absorption cross sections, and rate coefficients, are most conveniently written in CGS units. Some meteorological variables, such as wind speed, geopotential, and energy, are most conveniently written in SI units. Thus, both unit systems are retained. Unit and variable conversions are given in Appendix A.

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