Measurement Methods in Atmospheric Sciences

In situ and remote

Stefan Emeis

Quantifying the Environment

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with 103 figures and 28 tables

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Cover: Front cover: Radio-acoustic sounding system (SODAR-RASS) remotely ob-
           serving boundary-layer wind and temperature profiles up to several hundreds
           of metres above ground (see also Fig. 76). The three white acoustic antennas
           are seen behind one of the radio antennas in the foreground.
           Back cover from left to right: Radio-acoustic sounding system (SODAR-RASS,
           see also Fig. 76), open-path gas analyzer for CO_2 for turbulent flux measure-
           ments (see also Fig. 55), rain gauges with wind shields (see Fig. 34), Stefan
           Emeis (Photo: Sebastian Emeis).

Figures: All figures and graphs – unless otherwise stated in the legends – are from the
           author.

"I often say that when you measure what you are speaking about and express it in numbers, you know something about it, but when you cannot measure it, when you cannot express it in numbers, then your knowledge is of a meagre and unsatisfactorily kind; it may be the beginning of knowledge, but you have scarcely in your thoughts advanced to the stage of science, whatever the matter may be."

<div align="right">Lord Kelvin (1824–1907)*</div>

The malleefowl (*Leipoa ocellata*), an Australian megapode chicken, builds a nest from twigs and leaves in a up to 5 m wide and 1 m deep hole in the sand and covers it with sand. The bird keeps testing the temperature of the nest by dipping its beak into it. It influences the fermentation of the moist leaves in the nest by adding or removing some sand and thus keeps the temperature within the nest at constantly 33.5 °C.

<div align="right">www.world-of-animals.de/tierlexikon</div>

The snowy tree cricket (*Oecanthus fultoni niveus*) is also called a thermometer cricket because the rate of its chirps is temperature depending. Following Dolbear the temperature in °F can be determined by counting the number of chirps per minute, then subtracting 40, dividing the result by 4, and finally adding 50:

$$t\ [°F] = (n\text{-}40)/4 + 50 = (n/4) - 10 + 50 = (n/4) + 40$$

In centigrades the following approximation holds:

$$t\ [°C] = ((n/4) + 40 - 32)\ 5/9 = (5n/36) + 40/9 \approx (n/7) + 4.5$$

<div align="right">A.E. Dolbear (1897–1910)**</div>

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* From: Kelvin, W.T., 1889: Electrical Units of Measurement. In: Kelvin, W.T.: Popular Lectures and Addresses. Vol. I, Macmillan, London, 73.

** From Dolbear, A.E., 1897: The cricket as a thermometer. The American Naturalist, **31**, 970–971.
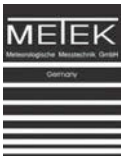
Preface

This book has emerged from lectures on meteorological measurement methods at the University of Cologne, Germany, both for students heading for meteorology as a principal subject and for graduated students heading for an International Master on Environmental Sciences (IMES). The teaching for both groups of students required to give a general overview of the large field of different measurement techniques which are available today to determine the state and composition of the Earth's atmosphere. The intention of these lectures was to convey the basic principles of the different observation and monitoring methods. Due to the large number of different measurement principles, it was not possible to describe single methods with a great depth. Additionally, many modern observation methods have become so complex, that a full description would nearly require a special series of lectures of its own.

The intention of this publication is to provide the reader with a manual which informs her or him on the available techniques of measurement, and if several methods are available, to give advices which method to choose for a given task. For this purpose, the lecture notes have been extended in several ways. First of all, more than 400 references, mostly to the recent scientific literature, have been added which will help the reader of this book to get deeper insight in the various methods. Furthermore, tables at the beginning of each major section in Chapters 3 to 7 serve for a quick reference to the different methods. Then, recommendations have been added after each major section which contain additional hints for the use of some instruments and which will facilitate the selection of a proper instrument for a given task. Finally, an appendix has been supplied which gives an impression of an additional body of literature which is often mandatory to be consulted when planning an observation or a monitoring task: national and international guidelines and standards. Today, the work of many bureaus of standards also covers a larger number of environmental monitoring techniques and gives precise information on the application of the instruments and the techniques of data evaluation in order to enable the acquisition of reliable and comparable data sets. A special index will help to use this information.

Many people encouraged and supported me during the compilation of the material for this book and helped with hints to further measurement methods, to special papers in the literature, and to illustrative material. First of all, my thanks go to the publisher who accompanied the preparation of the material with great interest from the very beginning and who offered this fine publication platform to me. Several colleagues from instrument manufactures read parts of the manuscript and gave valuable hints and supplied a few graphs. A great thank goes to Helmut Mayer, who read an earlier version of the complete manuscript, and even more important, who made his large collection of illustrative material available to me. Several of his photographs have been selected and will help the reader to better understand the measurement techniques. Nearly unestimatable is the support which a native English speaker can give an author who has grown up with a language different from English. Here, I experienced the great luck to get the help from Richard Foreman, who

diligently read the complete manuscript and who made an uncountable number of suggestions to improve the text.

Now, I hope, the book will be useful to its readers. As everybody knows, no one is perfect and a careful and experienced reader will easily spot those methods described in the book, with which the author is more acquainted than with others. Nevertheless, also with help of the many references included in the text, hopefully a fair and balanced overview on the presently available observation and monitoring techniques has been achieved. May the information gathered in this publication contribute a small piece to the making of a better and sustainable environment for all of us and those following us.

Weilheim, October 2009

Contents

1 Introduction

Without measurements we cannot gain any cognition on the exact state of our environment. This relates to the atmosphere as well as to all other compartments of the Earth's system. Taking a measurement is thus one of the most basic and elementary exercises in each science. This very fact in itself justifies a monography on meteorological measurement techniques and methods.

After the basics of air temperature, pressure, and moisture measurements have already been laid three to four hundred years ago, meteorological measurement techniques have seen a rapid development in the last few decades. Fostered by the progress in the development in electronics and computer technology, smaller and more complex measuring devices became available. At the end of the 1950s, in addition, a completely new measurement platform became available: satellites in orbits around the Earth. Based on this evolution an entirely new type of instruments came into existence: remote sensing devices. Today remote sensing techniques comprise a larger part of all meteorological observation techniques. Therefore nearly the same space as for the classical methods is devoted to remote sensing methods in the present book.

With the growing awareness for environmental protection a shift in observational needs has taken place compared with classical meteorology. Air quality and chemistry have become an important issue to observe and monitor. The spectrum of these new requirements ranges from acid rain and near-surface air pollution to stratospheric ozone loss and the still undamped increase of the concentration of greenhouse gases in the Earth's atmosphere. This justifies separate chapters on the measurement of atmospheric trace gases and aerosols to be included in this book.

Since the last two centuries has seen an advancing specialisation in meteorology as in most other scientific disciplines, it now becomes more and more obvious that only a joint consideration of all compartments of the biogeochemical system Earth is meaningful. This includes the observation of exchange processes between these compartments. For example, the growing importance of monitoring exchanges between the atmosphere and its underlying surface has recently increased once again the interest in micrometeorology and its special observational skills. Here, the focus is especially aimed on the direct measurement of turbulent fluxes of carbon dioxide and water vapour. Although monographs on micrometeorology exist, micrometeorological methods must be a part of any general overview on meteorological observational techniques.

A few monographs on observational techniques for the atmosphere are available today which aim at a similar completeness as the classical book by Kleinschmidt (1935), e.g. "Meteorological Measurement Systems" by Brocks & Richardson (2001), Strangeways' "Measuring the Natural Environment" in a second edition

from 2003, "Surface Meteorological Instruments and Measurements Practices" by Shrivastava (2008), and the latest edition of the WMO "Guide to Meteorological Instruments and Methods of Observation" (WMO 2008) appeared recently. Strangeways' book predominantly concentrates on classical techniques emphasizing some hydrological aspects; Brocks & Richardson (2001) likewise concentrate on classical meteorological techniques, while the WMO publication quite naturally focuses on the needs of the weather services, as does the publication by Shrivastava.

Therefore the present book tries to offer a more comprehensive review on atmospheric measurement techniques within which air chemistry, remote sensing, and micrometeorology are given the necessary space they require today. However, remote sensing is still a field of rapid development of which no final, ultimate description of all relevant measurement techniques can be provided here. The remote sensing methods introduced here rather represent a snapshot of the present state of development. The book intends to present an overview of the large variety of instruments and their basic operational principles. There is no space to go into technical details of single instruments which may even change from manufacturer to manufacturer. Such details for single classical meteorological instruments for surface observations can be taken from, e.g. WMO (2006) and Shrivastava (2008). A large number of references and the list of guidelines and standards in the Appendix will help the reader to find more details on special instruments and methods.

Data acquisition and storage is a task which is nowadays nearly completely automated. Thus, these two tasks will be given only minor consideration here. This however, should not be interpreted as an invitation to use the available hard- and software for data management without a critical perspective. The emphasis of this book will therefore be on the basic principles behind the measurement techniques. The knowledge on these techniques is a prerequisite for reliable interpretation of data.

1.1   The necessity for measurements

Observation is a cornerstone for gaining cognition and understanding in all sciences. Measurements quantify observations. Quantifying data acquisition has been the precondition for all modern natural sciences and thus also for physics and meteorology. Knowledge on past and present processes taking place in the atmosphere can only be obtained by observations and measurements. Likewise, measurements lay the foundation for any forecast of future events, and only measurements will permit later tests of the accuracy and precision of these forecasts. Just as well, measurement techniques and methods are the prerequisite for experimental studies in order to improve our understanding of selected processes.

In applied meteorology, measurements are necessary for analysis, monitoring, and documentation of the present weather and climate, as well as for the acquisition of initial and input data for models of weather and climate predictions. Likewise, they are needed for assessment and for monitoring air quality and to check for com-

plience with the given threshold and limit values. In meteorological research, measurements are mandatory for any further enhancement of the knowledge. All these tasks demand high-quality measurement devices. More rigorous research and monitoring demands are the main driving force for the ongoing development and refinement of measurement techniques and instrumentation.

1.2   Definition of a measurement

Measurements aim at a quantitative determination of the state of a system (in meteorology this system is usually the atmosphere or a part of it) with respect to selected thermodynamic, kinetic, and chemical state variables. For an ideal gas such as dry air e.g. two of the three basic state variables pressure p, volume V, and temperature T must be determined. Then the thermodynamic state of this gas is known because the third variable can be computed from the law for ideal gases ($pV = RT$ with the gas constant R). In order to assess the kinetic state of a gas, its movement has to be determined, i.e. the spatial distribution of the three velocity components must be measured in a gas volume. Its chemical state can be inferred from an analysis of the chemical composition of the gas. For a description of the temporal evolution or for a forecast of a system, the knowledge of internal conversion rates and of energy and mass fluxes across the outer boundaries of the system have to be known. These include, e.g., the incoming solar radiation, the outgoing thermal radiation, mass fluxes such as falling precipitation, or turbulent vertical fluxes at the Earth's surface.

To be very precise, a measurement is performed by comparing a selected state variable of the system in question (pressure, temperature, etc.) with a predefined scale for this variable (Pascal for pressure, Kelvin for temperature, etc.). This comparison yields a number indicating how often the selected scale is contained in the measured quantity. Or putting it differently, this number establishes a relationship between the state of the observed system and a selected system of reference which serves as a scale.

Practically, a measurement is performed by operating a measuring device. These devices capture the physical or chemical state of the observed system in a suitable way and perform (usually after a gauging or calibration procedure) the above mentioned comparison. To define what is best suited will be the main task of the present book.

The recorded number or measurement value obtained from a measurement cannot be judged independently of that particular measurement technique or method. Peculiarities and limitations of the technique must be known. These comprise, e.g., the temporal and spatial resolution of the data measured with a given instrument. Variations of the measured value smaller than the resolution of the instrument cannot be assessed. Or to put it in another way: a fishing net with a 5 cm mesh size will catch only fish larger than 5 cm (Dürr 1988). Principally, a measuring instrument will only deliver information on processes for which it has been designed.

Measurement of all relevant state parameters of a system results in a set of numbers (parameters) which characterizes and parameterizes the system. This does not necessarily imply a complete description of this system because a choice of what is relevant has been determined or – using the net analogy introduced above – a fishing net with a predefined mesh size has been employed.

1.3   Historical aspects

Quantifying instruments have been known for about 400 years. For information from the time before the invention of modern instruments, one had to rely on "proxy data". These are observations of facts and circumstances which are related to the sought after variable in some, mostly not very precise way. Proxy data include, e.g., the width of tree rings, carbon and oxygen isotope ratios in organic matter, data on harvesting and floods. We will not address the methods to survey and evaluate proxy data in the present book.

The still ongoing development of instruments, that deliver quantitative and reproducible data, started in the period of the renaissance in the 17th century. During the past 30 years, semiconductors and microelectronics have been offering entirely new perspectives. Today, progress in computer technology and storage media permit nearly completely automated measurements, the storage of vast amounts of data, and online evaluations. The precision and resolution of many observational methods has been enhanced considerably – and at the same time – the efforts for maintenance reduced drastically.

Today, in addition to the classical methods which require the direct proximity of the instrument to the object of investigation, remote sensing techniques gain an ever larger part of the usual measurement techniques. The development of remote sensing instruments has been the prerequisite for the use of new platforms like orbiting satellites. This development has only been possible because mathematical methods such as Fast Fourier Transforms furnished the necessary evaluation techniques. These rapidly operating mathematical tools are necessary because of the indirect nature of remote sensing methods which just record irradiance data: classical meteorological or air quality variables can only be isolated by laborious inversion techniques from remote sensing data. But also classical measurement methods – as the next chapter will show – nearly always involve inversion procedures. However, these inversions are, in most cases, an integral part of the method, either by the technical design of the instrument or by gauging and calibration procedures, and are therefore often not obvious to the users.

Milestones of measurement instrument development have been among others the following developments (for a detailed overview on the invention of meteorological instruments until the middle of the 20th century see Middleton 1969):

Fig. 1. Kite used by the meteorological observatory in Lindenberg, Germany, for meteorological measurements throughout the whole troposphere at the beginning of the 20th century.
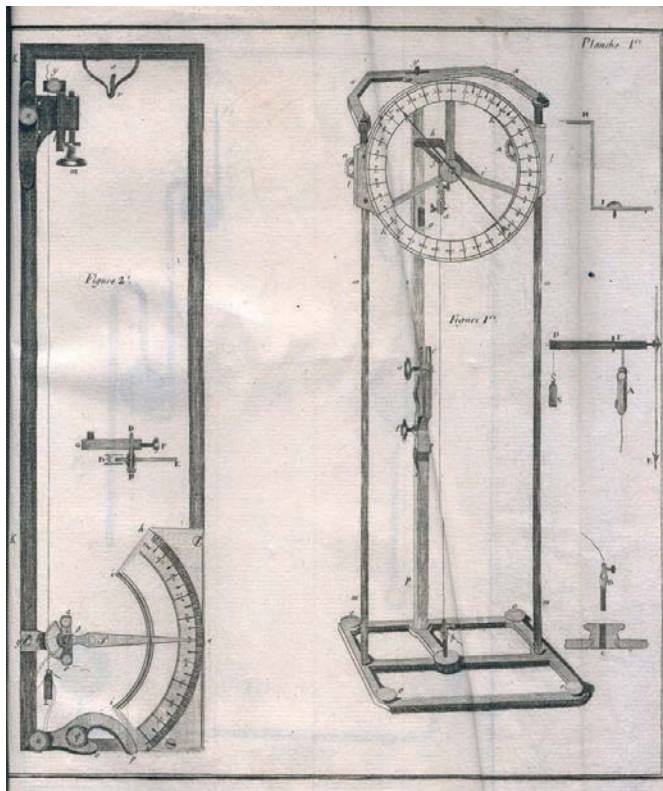
Fig. 2. Drawing showing Saussure's hair hygrometer. Left: the length change of the hair is directly transferred to the pointer (at the lower end of the instrument), right: length change is translated to a clockwise rotating pointer (to the top of the instrument). Source: Saussure (1783), http://orpheus.ucsd.edu/spec-coll/weather/b4161877.html (Official Web Page of the University of California San Diego, Copyright 2007, UC Regents).

1593 Galilei's thermoscop (a precursor of the thermometer)

1643 Torricelli's mercury barometer

1654 first meteorological observational network in the Tuscany

1749 first scientific kite ascent (see Fig. 1)

1783 Saussure's hair hygrometer (Saussure 1783, see Fig. 2)

1783 first meteorological measurements during a balloon ascent (first vertical profiling)

1843 Vidie's aneroid barometer

1846 Robinson's wind speed meter

1853 Campell's prototype of the sunshine autographe

1886 first alpine mountain observatory (Hoher Sonnblick, Austria)

1921 first ozone column density measurement with a spectrometer (first remote sensing)

1930 first radiosondes (first regular vertical soundings)

1947 first weather RADAR (first regular detection of precipitation)

1960 first meteorological satellite (first sounding of the Earth's atmosphere from space)

1975 first wind profiler (advancement of ground-based remote sensing)

1979 first DOAS (advancement of optical remote sensing)
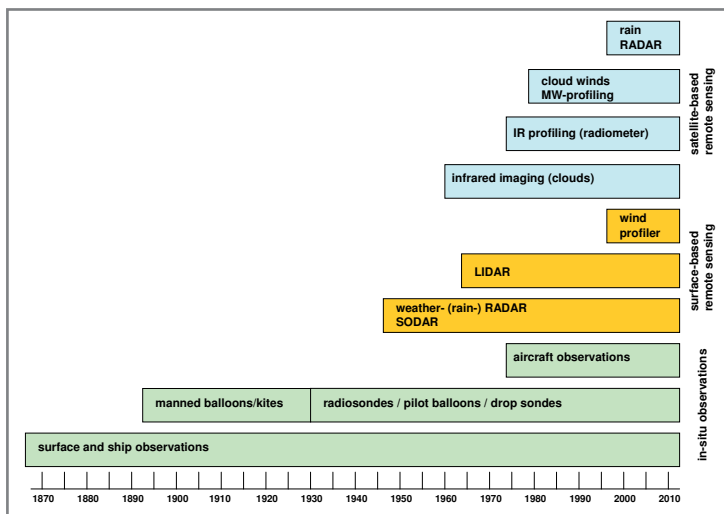
Fig. 3. Timeline of routine weather observation techniques (extended from Uppala et al. 2005) showing in-situ techniques in the lower three bars, surface-based remote sensing techniques in the middle, and satellite-based techniques in the upper four bars.

Figure 3 shows in schematic form the temporal development of routine meteorological measurement methods for monitoring and the provision of input data for numerical weather forecasts.

2 Measurement basics

2.1 Overview of methods

This chapter introduces the basic characteristics of measurement techniques and methods described in this book.

2.1.1 Direct and indirect methods

A direct measurement consists of a direct comparison of the object which is to be studied with a given scale. This simple approach is applicable only for length, mass, and time measurements. A length measurement is accomplished by holding a meter stick directly to the object in question. A time measurement is performed by direct comparison with a clock. A mass determination is made by applying the correct counterweight to the other side of a pair of balances.

All other measurements are carried out indirectly and are based on the observation of how the measurement variable of interest influences or modifies an appropriate sensor. Watching the modifications of the sensor gives indirect access to the variation of the variable of interest. E.g. a radiation measurement is usually based on the observation of how a black plate, which is used as a sensor, heats up or cools down. In this sense, nearly all methods covered in this book are indirect methods. The only exceptions are the three direct methods described above. Mathematically speaking, indirect methods involve an inversion procedure.

2.1.2 In-situ and remote sensing methods

During an in-situ measurement, direct contact prevails between the sensor and the object whose properties are to be determined. This in turn has the consequence that every in-situ measurement influences the object during the measurement. One of the challenges in instrument development is to design it so that repercussions of the instrument on the object are as small as possible. Measuring the air temperature with a thermometer which initially has a temperature different from that of the air will inevitably slightly change the air temperature. Thus the measured temperature is no longer the 'true' air temperature just before the measurement. This repercussion is proportional to the mass ratio of the sensor to the air volume whose temperature is to be determined. Therefore minimizing the size of a sensor is usually a good means to reduce repercussions of sensors on the observed systems.

During remote sensing measurements there is no direct contact between the instrument and the object and repercussions are unlikely. Remote sensing analyses the radiation scattered back or emitted from an object or transmitted through that object. The measurement can be complicated by further modifications of the radiation between the observed system and the instrument. Generally, a radiative transfer equation has to be solved in order to complete the measurement. Passive remote sensing, a method that passively monitors the radiation emitted from a system or transmitted through it, does not influence the observed system at all. Active remote sensing, which is based on the reception of backscattered radiation of a well-defined signal that had been emitted before by the measurement device, could have slight but usually unimportant repercusions on the observed system. The great advantage of remote sensing is that it can aquire information on systems not accessible for in-situ measurements. This comprises, e.g., systems that are unreachable because they are too high above the ground or systems whose state does not permit in-situ measurement (e.g., because they are too hot).

Remote sensing can be performed in several modes: the most important modes are sensing, sounding, scanning, and imaging (see also Fig. 63). Sensing just monitors the instantaneously oncoming radiation. Sounding is based on the emittance of a pulse and the subsequent detection of backscattered radiation during a given time window. Scanning means that the receiving detector is repeatedly turned into different directions in order to detect the incoming radiation. Finally, imaging involves the operation of a focussing element which projects the incoming radiation on a horizontally resolving detector array. Classical photography was the first optical imaging method. Sounding and scanning can be combined, see, e.g., the weather RADAR below.

2.1.3   Instantaneous and integrating methods

Instantaneous measurements are performed in parallel to real processes and yield a momentary value or a series (e.g., time series). The time resolution depends on the sampling rate and the inertia of the sensor.

Integrating measurements either accumulate the impact on the sensor over a longer time period (e.g., daily precipitation sums) or they average over a larger number of instantaneous measurements (e.g., eddy correlation flux measurements). Averaging over many instantaneous measurements is advisable if single measurements have a large associated statistical uncertainty. The averaging procedure then helps to enhance the signal-to-noise ratio.

2.1.4 On-line and off-line methods, post-processing

Both in-situ and remote sensing measurements are mostly on-line methods, i.e. sampling and analysis are made at the place for which and from which the information is needed. This is true for instantaneous as well as for integrating methods.

Some measurement methods are so laborious that they cannot be performed on-line. Post-processing of the obtained data is either very time consuming or needs special boundary conditions in order to deliver reliable results. In these cases raw data are stored and later processed in the laboratory. An example for such a post-processing is the chromatographic analysis of the detailed chemical composition of air collected in special containers. Often off-line methods permit much lower detection limits, i.e. smaller concentrations can be analysed more reliably.

2.1.5 Flux measurements

In many cases characterization of a system does not only require knowledge of state variables such as temperature, density, or trace gas concentration in the interior of the system but also of fluxes of matter or energy across the boundaries of the system. A flux is defined as the amount of a substance, energy, or – more generally – a property which passes per unit time through a unit area. Within the Earth's system, e.g., these can be fluxes from one compartment (atmosphere, ocean, cryosphere, soil, etc.) of the system to another.

The usual transport velocity of substances (gases or aerosols) or energy and momentum is the wind speed. Exceptions are sedimenting atmospheric constituents like rain drops and non-material fluxes of radiation energy. Let A be a surface area, v_a a velocity perpendicular to this surface A, and e a property of the atmosphere. The momentary flux of this property F_e is given by:

$$F_e = \frac{1}{A} v_a e \tag{2.1}$$

Now, an overbar ($\overline{\ldots}$) denotes a spatial or time mean value (ensemble average) and a prime (') a deviation from this mean (fluctuation), then the flux F_e can be splitted into a mean flux $\overline{F_e}$ and a turbulent flux F_e':

$$F_e = \overline{F_e} + F_e' = \frac{1}{A} \overline{v_a}\,\overline{e} + \frac{1}{A} \overline{v_a'e'} \tag{2.2}$$

The measurement of mean fluxes $\frac{1}{A} \overline{v_a}\,\overline{e}$ which are coupled to atmospheric mean motions is relatively simple. It just requires the determination of the mean wind speed $\overline{v_a}$ and the mean value of the property $\overline{e}$ integrated over the area A and a subsequent multiplication.

The mean flux $\overline{F_e}$ is not always the most important contribution to the total flux F_e. Especially close to the surface, the turbulent part F_e' can be considerably larger than the mean part due to the imperviousness of the ground surface. Simultaneously,

mechanical (shear) and thermal (buoyancy) generation of turbulence near the surface lead to larger fluctuations of the vertical velocity around its vanishing mean value. If also the property e whose flux is to be determined exhibits larger fluctuations and if these fluctuations are correlated with vertical wind fluctuations, then we will observe a large turbulent flux without any mean mass flux. Especially at the boundary between the Earth's surface and the atmosphere, these turbulent fluxes play a prominent role in the global mass and energy budgets. Therefore Chapter 6 is devoted to flux measurement methods.

The direct measurement of turbulent fluxes requires the simultaneous measurement of wind and property fluctuations with high temporal resolution. Subsequently, the covariance $\overline{v_a'e'}$ between the two time series of fluctuations has to be computed from the raw data in order to determine the turbulent flux. The measurement of turbulent fluxes is one of the main tasks of micrometeorological methods described in Chapter 6.2 in more detail.

2.2   Main measurement principles

In order to characterize the properties of a measurement method we must understand the main steps executed during the data acquisition. The principle sequence is as follows: A sensor or detector records the input signal. The signal is then transformed and/or amplified within the measurement device. Finally, the transformed output signal is shown on a display (either analogue or digital) and/or written to a storage medium (see Fig. 4). Most instruments need some auxiliary energy supply to perform recording, transformation and display or storing of the information. This energy can be supplied either mechanically (e.g. by a clockwork) or electrically.
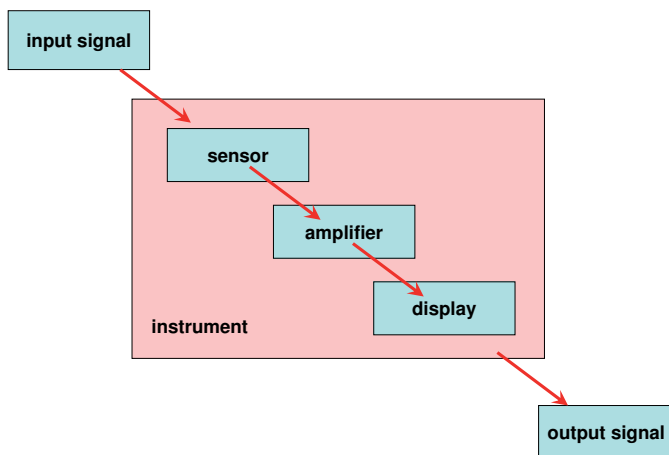

Fig. 4. Basic operation principle of a measurement instrument detecting an input signal and producing an output signal. Instruments usually comprise a sensor, an amplifier, and a display.

input signal

21

20

19

18

output signal
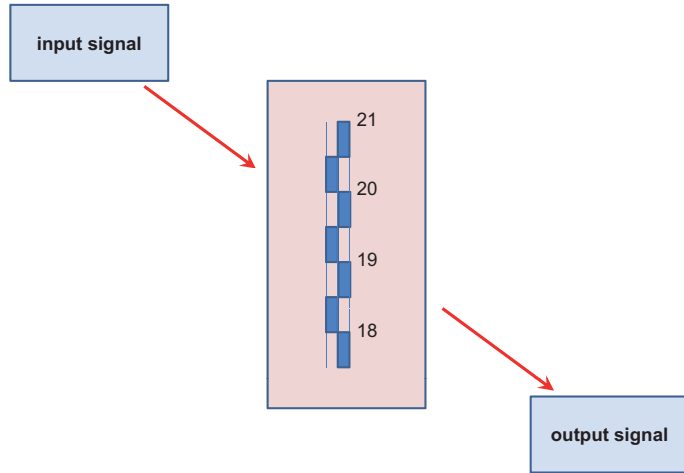
Fig. 5. Schematic of a length measurement with a meter stick as example for a direct measurement.

The simplest example is measuring the length of an object with a meter or yard stick. This stick combines all three functions (sensor, transformer, display) in itself (Fig. 5). The length of the object can directly be read off the scale engraved on the meter stick brought next to the object.

Determining the temperature of an object is somewhat more complicated (Fig. 6). Let us have a look at the classical liquid-in-glass thermometer. The sensor for the air temperature is the thermometric liquid (usually alcohol or mercury) which is captured in the glass container of the thermometer. This glass container acts as an amplifier because the change in length of the liquid thread in the capillary tube depends on the ratio of the width of the capillary tube and the thermometer bulb (see also Fig. 7). The thinner the capillary tube the more sensitive is the thermometer. The display

input signal

amplifier

30
20
10
0
-10
-20
-30

display

instrument

sensor

output signal
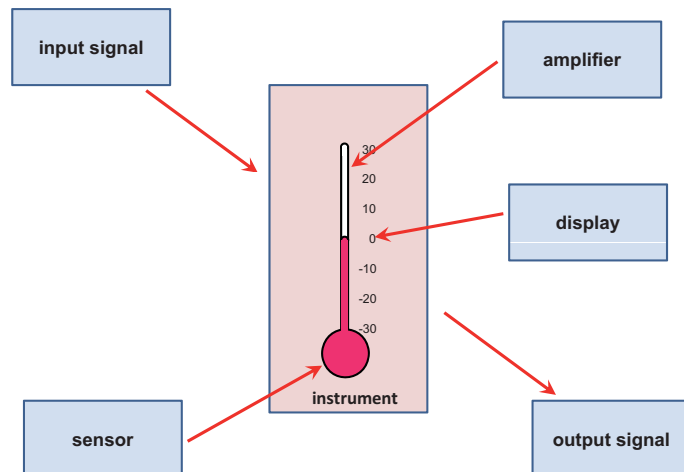
Fig. 6. Schematic of a temperature measurement with a liquid-in-glass thermometer as example for an indirect measurement.
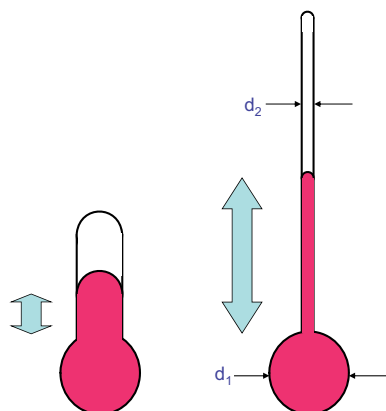
Fig. 7. Mechanical amplification of the temperature signal in a liquid-in-glass thermometer. The amplification is proportional to the ratio d_1 (diameter of the bulb) to d_2 (diameter of the capillary tube). Left: low amplification, right: high amplification.

of the thermometer is the capillary tube to which a scale is attached. Reading the length of the liquid thread in the capillary tube in itself is a direct length measurement as described above.

This makes obvious that the process of obtaining the temperature of a system is an indirect measurement method. The internal energy of the system acts on the thermometric liquid and changes its volume. By the way the thermometer is constructed this volume change of the liquid is translated to a length change of the liquid thread, and finally, this length is read by comparing it to a length scale. Once a thermometer has been built, the scale has to be adjusted to this very thermometer by calibrating it. This calibration process also compensates for effects of the slight change of volume of the glass container of the thermometer with temperature.

2.3   Measurements by inversion

As just discussed, most measurement methods are indirect methods and therefore require an inversion to obtain the sought atmospheric variable from the recorded raw data. The following aims to provide a short introduction to the main idea of inversion. This digression is not fundamental for the understanding of the rest of the book but it is presented here to provide an insight into such formalism. In a much more complex manner, an inversion is a constitutional part of such methods as emission rate determination (Ch. 6.6), remote sensing methods (Ch. 7), and tomographic methods (Ch. 7.5).

2.3.1   Inversion with one variable

Once again the measurement of the temperature of a system with a classical liquid-in-glass thermometer shall serve as an example. Mathematically speaking, a temperature measurement is a mapping which can be expressed by a function *g*:

$$m = g(z) \tag{2.3}$$

Function g in (2.3) maps the state variable internal energy, z of the observed system to the measured value, m. Generally, z and m are vectors, but in our example they are just scalar quantities. If the state variable z and the function g are known, the measured value m can be predicted. This is also called forward modelling. Taking a measurement is just the reverse operation: here the measured value m is determined by reading the instrument and we must invert the process described by the function g in order to get the atmospheric state variable z. Mathematically this reads:

$$z = g^{-1}(m) \tag{2.4}$$

As we execute the model described by the function g in an inverse way, the procedure (2.4) is also called inverse modelling. To elucidate this inversion procedure we will specify the functions g and g^{-1} for the liquid-in-glass thermometer. As discussed in Chapter 2.2, measuring the temperature T is a two-step procedure, and therefore we must split the model described by the function g in two parts g_1 and g_2. g_1 mirrors the effect of the internal energy of the air $z = c_v T$ on the volume, v of the thermometric liquid and g_2 transforms the volume change of the liquid, $v(T) - v(T_0)$ to the length change of the liquid thread, $l - l_0$ in the capillary thread:

$$g_1: v(T) = v(T_0)(1 + \gamma(T - T_0)) \tag{2.5}$$

with the thermal expansion coefficient, γ of the thermometric liquid and the temperature, T in K, and:

$$g_2: l = l_0 + \lambda(v(T) - v(T_0)) \tag{2.6}$$

with the constant, λ which has the dimension m^{-2} and which depends only on the construction of the glass container of the thermometer. l_0 is the length of the liquid thread at temperature T_0.

The length of the liquid thread is measured directly (expressed by a function d) by reading the scale fixed at the thermometer. The complete concatenated forward model for a temperature measurement reads:

$$m = d(l) = d(g_2(v)) = d(g_2(g_1(T))) \tag{2.7}$$

Inserting (2.5) and (2.6) in (2.7) we obtain for (2.3):

$$m = d(l_0 + \lambda(v(T_0)(1 + \gamma(T - T_0)) - v(T_0))) = d(l_0 + \lambda\gamma v(T_0)(T - T_0)). \tag{2.8}$$

As we need (2.4) instead of (2.3) we now have to perform an inversion. The inverse of the direct observation d^{-1} is identical to d itself. For functions g_1 and g_2 it has to