Thesis for the degree of Licentiate of Engineering

Remote sensing of ice clouds and precipitation from active and passive microwave observations

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Gosto de um modo carinhoso do inacabado, do malfeito, daquilo que desajeitadamente tenta um pequeno vôo e cai sem graça no chão.

— Clarice Lispector

Abstract

Keywords: Micro wave remote sensing, frozen hydrometeors, precipitation, clouds

Acknowledgments

Simon Pfreundschuh
Göteborg, November 2019

List of Publications

This thesis is based on the following appended papers:

Paper ??. Cool paper

Other relevant publications co-authored by Simon Pfreundschuh:

Another cool paper

List of Acronyms

IWC – Ice water content

Contents

Part I

Introductory chapters

Chapter 1

Introduction

Clouds and precipitation affect live on Earth in multiple ways and on multiple time scales. On short time scales, weather affects human activity, potentially posing threats to transport, agriculture and lives. On longer time scales, precipitation patterns shape ecosystems and societies while clouds influence the global climate system through their interaction with the incoming and outgoing electromagnetic radiation.

As historical evidence suggests, understanding and predicting weather and climate has been a human endeavor dating back at least to the formation of the first settled communities during the agricultural revolution. This is not surprising considering the dependence of agricultural activity on benign weather patterns. Today, this dependency has likely even increased as more and more branches of human activity rely on the availability of reliable weather forecasts.

As the dramatic effects of anthropogenic climate change become more and more apparent (Coronese et al. 2019; Grinsted et al. 2019), the importance of understanding and predicting the Earth's changing climate is indisputable. The predicted heating under all but the lowest emission scenario is likely to exceed 2 °C by the end of the century (Collins et al. 2013). With this, global mean surface air temperature will become higher than what has can be estimated from reconstructions of past climate (Masson-Delmotte et al. 2013).This only underlines the importance of a thorough understanding of the processes that govern climate change on Earth.

The subject of this thesis are observational methods for clouds using microwave sensors. These observations provide valuable information on the state of the atmosphere for weather prediction as well as a basis for the evaluation and improvement of climate models. The remainder of this introduction aims to give an overview over the relevance of observations of clouds for both weather and climate prediction and closes with a discussion of currently available observation methods. The following chapters then provide an introduction to physical and mathematical principles upon which these observations are founded. Chapter 2 provides an introduction to cloud formation and establishes what properties of clouds can be observed. Chapter 3 introduces the theory of radiative transfer which describes how radiation interact with clouds and which is necessary to understand the observable effects that clouds have on microwave radiation. Finally, Chapter **??** introduces the mathematical methods that are used to infer clouds properties from observations of clouds.

A brief remark on the terminology: Clouds and precipitation consist of particles formed by frozen or liquid water. Hydrometeor is used in the following as a collective term to denote either of these forms. Moreover, the adopted viewpoint is that precipitation is a byproduct of cloud formation and therefore the terms 'observations of clouds' or 'cloud observations' are used to denote observations of both clouds and precipitation.

1.1 The role of clouds and precipitation in numerical weather prediction

Clouds and precipitation are responsible for many of the phenomena that are considered as weather. It should therefore be clear that their accurate representation in numerical weather prediction (NWP) models is essential for reliable forecasts. But clouds, more specifically observations of clouds, can impact weather forecasts in another, more nuanced way.

Modern forecasting systems make use of satellite observations to determine an optimal initial state from which a forecast run is started. This process is called data assimilation. In a clear atmosphere, satellite observations from the infrared and microwave domain can provide direct information on the temperature and humidity field of the atmosphere. When observations are assimilated over multiple time steps, sequences of observations can provide additional information on wind speeds (Alan J. Geer et al. 2018). In a cloudy atmosphere, satellite observations still provide information on temperature and humidity, but in addition to that the presence of clouds can provide information on the dynamical state of the atmosphere.

Clouds form where warm and moist air is transported upwards in the atmosphere by convection. Cloud formation thus acts as a tracer of atmospheric dynamics that can provide valuable information on the state of the atmosphere. Indeed, owing to recent developments in data assimilation methodology, microwave observations sensitive to humidity and clouds have become a main contributor to short-term forecast skill (A. J. Geer et al. 2017).

1.2 The role of clouds and precipitation in the climate system

The main impact of clouds on the climate system is through their interaction with the incoming solar radiation and the outgoing long-wave radiation, which determines the Earth's energy Budget. In addition to that, clouds form a part of the global hydrological cycle in which they deliver water from the atmosphere to the surface of the Earth.

1.2.1 The global energy budget

The short-wave radiation emitted by the sun that reaches the earth is the energy source that drives the climate system. To remain at a stable temperature the Earth needs to emit the same amount of incoming energy in the form of outgoing long-wave radiation. From an energy balance perspective, clouds have two opposing effects on the global energy budget. The first one is a cooling effect caused by the reflection of incoming short-wave radiation back to space. The second effect is a warming effect caused by the blocking of outgoing long-wave radiation that would be emitted to space in a cloud-free atmosphere. Overall, the cooling effect of clouds prevails, leading to net cooling effect of clouds.

1.2.2 Cloud radiative effect and climate sensitivity

Since both the cooling and warming effects of clouds are relatively strong, changes in cloud properties or occurence may potentially cause significant feedbacks in a changing climate. These effects, however, are difficult to quantify. This is because the strength of their interaction with radiation depends on where clouds form in the atmosphere as well as on their microphysical properties such as particle phase and size distribution. Furthermore, the formation of clouds involves size-ranges beginning at the nanometer scale of aerosol particles on which cloud drops form up to several thousands of kilometers, which is the size of synoptic-scale cyclones. This wide range of size-scales is very difficult to represent in global climate models, which is why they have to rely on approximate representations of cloud processes.

The cloud feedback is indeed the most uncertain feedback affecting the global climate. It therefore contributes significantly to the spread in predicted changes in global mean surface temperature observed between different GCMs.

1.3 Global observations of clouds

The two previous sections described the relevance of cloud observations for weather and climate applications. This section provides a brief review of common, global observation methods for clouds. The focus here is put on satellite-based observations since these are the only ones that can provide observations at global scales and temporal resolutions.

1.3.1 Frequency domains

Hydrometeors can be observed from the optical domain down to microwave frequencies around 10 GHz. The strength of their interaction with radiation is determined by the relation of their size to the wavelength of the radiation, which is strongest when the wavelength is close to the particle size.

In the optical and infrared, cloud droplets and ice crystals are large compared to the wavelength of the radiation, so the interaction with a single particle is not very strong. However, the large number concentrations of these particles make clouds opaque at these wavelengths. This has important implications for cloud observations using optical or infrared radiation. Since the cloud is opaque the observed radiation is sensitive only to the upper-most regions of the cloud. Observational techniques based on these wavelength therefore have no direct sensitivity to precipitation and large parts of the water masses in thick clouds.

At microwave frequencies, the wavelength of the radiation is much larger than the size of the hydrometeors rendering microwave radiation insensitive to all but the largest hydrometeors. The advantage of microwave observation is that they can directly sense precipitation, which occurs in clouds that are too thick for optical or infrared radiation to penetrate.

A considerable gap in observation wavelengths between the highest microwave frequencies around 2 mm and the lowest infrared observations at around 15 μm. This gap is due in part to the strength of the water vapor continuum in this region of the electromagnetic spectrum, which makes the troposphere invisible from space for large parts of it. Another reason are technological difficulties in the development of sensors for these wavelengths.

1.3.2 A look into the future

Nonetheless, progress is underway to close this frequency gap. The Ice cloud imager (ICI) will be flown on the upcoming second generation of European operational meteorological satellites (Metop-SG) and will provide observations of the atmosphere at frequencies up to 664 GHz corresponding to a wavelength of less than 0.5 mm. These observations at sub-millimeter wavelength will considerably increase the sensitivity to small particles and lower hydrometeor masses.

For the observations provided by ICI to be useful the development of additional know-how and methodology is required. This is mainly because the microphysical properties of ice, i.e. their shape and size affect the observations at these high microwave frequencies. The development of methods to infer cloud properties such as the mass density of hydrometeors from these observations thus requires consideration of these microphysical properties. These developments are also the main topic for the PhD project that lead to this thesis.

Chapter 2

The physics of clouds and precipitation

Clouds consist of large numbers of water droplets and ice crystals that are suspended in the air. When these drops grow sufficiently in mass they eventually fall out of the cloud to form precipitation. This chapter gives an overview over the processes that lead to the formation of clouds and ultimately precipitation. Moreover, the typical properties of the hydrometeors that make up clouds and precipitation are presented. This knowledge is required to understand the capabilities and limitations of the observational approaches in the remainder of this thesis.

It is common to classify cloud types according to their form which is representative of the dynamical context in which they form. Such a classiflication is of minor relevance for the development of observation methods of clouds and is therefore not presented here. Instead, warm and cold clouds are distinguished. Warm clouds exist below the 0 °C isotherm and consist solely of liquid water droplets. Cold clouds extend to above the 0 °C isotherm consist at least in part of ice particles. Although, typically, the liquid phase is present also in cold clouds, this classification allows the slightly different formation processes of liquid and frozen hydrometeors to be discussed separately. Moreover, also the signature of liquid and frozen hydrometeors in remote sensing observations are farily, which is why observation methods for different types of hydrometeors are generally considered separtely.

This chapter begins with an introduction to phase transitions and how they are initiated to form clouds. Then the formation of cloud is discusses separately for warm and cold clouds. The chapter closes with a brief discussion of the general properties of precipitation.

2.1 Principles of cloud formation

Cloud hydrometeors form when the water vapor contained in the air undergoes a phase change from the gas phase to the liquid or frozen phase. These processes are denoted as condensation, for the change from the gas to the liquid phase, and deposition, for the change from the gas to the ice phase. Their inverse processes, i.e. the change from water in the liquid respectively ice phase to the gas phase are denoted as evaporation and resublimation.

A necessary condition for condensation to occur is that the air is supersaturated with respect to liquid water. This means that the partial pressure of water vapor exceeds the saturation vapor pressure with respect to liquid water. Similarly, supersaturation with respect to the ice phase is required for the formation of ice particles. The supersaturation required for the formation of clouds is reached when comparably warm and moist air is lifted in the atmosphere. The resulting adiabatic cooling of the air leads to a decrease in the saturation vapor pressures of water and ice and the air eventually becomes supersaturated.

When water vapor reaches supersaturation with respect to either the liquid or ice phase it enters a metastable state. This means that although the liquid state is energetically favorable the transition is inhibited by an energy barrier. Due to the random nature of the movements of water vapor molecules, some of them eventually overcome the energy barrier by forming clusters of the new stable phase inside the metastable gas phase. In the context of phase transitions, this process of forming clusters of the stable state inside the metastable parent state is referred to as nucleation. More specifically, two types of nucleation are distinguished: Homogeneous nucleation refers to the process of forming a new, pure cluster of molecules in the stable phase whereas heterogeneous nucleation refers to the formation of a cluster of molecules in the stable phase on or around a cluster of a different molecular species.

After a sufficiently large nucleus has formed, it will grow due to the condensation or deposition of water molecules as long as its environment is supersaturated with respect to its phase. Eventually, differences in fall velocities between particles of different sizes will cause the particles to collide and stick together which further accelerates particle growth.

Due to the different molecular properties of water and ice, slightly different processes are involved in the formation of liquid cloud droplets and ice particles, respectively. These together with the corresponding growth mechanism are explained in more detail in the following two sections.

2.2 Warm clouds

As has been mentioned above, warm clouds are clouds that do not extend above the 0 °C isotherm and consist solely of liquid cloud droplets.

2.2.1 Formation

The formation of cloud droplets by homogeneous nucleation is highly unlikely due to the height of the energy barrier separating the metastable gas phase from the liquid phase. Instead, cloud droplets form through the activation of cloud condensation nuclei (CCN). CCN are soluble aerosol particles, which take up water molecules and grow even in environments that are not super-saturated. The droplets which are formed by hygroscopic growth of aerosol particles are called solution droplets. For sufficiently high supersaturations, the energy barrier for the transition to larger cloud drops vanishes leading to immediate condensation of all water molecules onto the droplet that are available in its surroundings. The theory describing the activation of CCN and their growth to cloud droplets is know as Köhler theory (Köhler 1936).

2.2.2 Growth processes

The condensation of water molecules onto the newly formed cloud causes a gradient in the concentration of water molecules initiating a diffusive flow of water vapor towards the droplet. The water vapor flowing towards the droplet condenses onto it making it grow in size and mass. This process is called growth by diffusion and condensation. The rate of diffusional growth decreases with increasing droplet radius. From sizes around 10 or 20 μm and up therefore another growth process takes over.

When the cloud droplets have grown sufficiently in mass, differences in fall speed between cloud droplets of different size as well as turbulence may cause droplets to collide. If these droplets coalesce the resulting droplet will have grown compared to the two colliding droplets. The resulting, larger particle will fall even faster down through the cloud. Heavier particles typically are also more efficient in collecting other cloud droplets. This illustrates why collision-coalescence is a very efficient growth process. Only collision-coalescence can explain the onset of rain only 20-30 minutes after the formation of a cumulus cloud which can be observed in the atmosphere.

2.3 Cold clouds

Cold clouds extend to above 0 °C isotherm and are characterized by the presence of frozen hydrometeors.

2.3.1 Formation

In contrast to liquid droplets, both homogeneous and heterogeneous nucleation are relevant for the formation of ice particles in the atmosphere. In agreement with Oswald's rule of stages, homogeneous nucleation occurs only through the liquid phase due to the prohibitively high energy barrier associated with the formation of an ice nucleus directly from the vapor phase. This means that ice particles are formed by homogeneous nucleation through the formation of an ice nucleus inside an existing cloud or solution droplet and subsequent complete freezing of the droplet. Nonetheless, the energy barrier for homogeneous nucleation of ice particles remains sufficiently high so that these processes occur only at temperatures below -36 °C for solution droplets and -38 °C for cloud droplets.

Heterogeneous nucleation of ice particles involves aerosol particles, so called ice nucleating particles (INP), that provide a surface onto which the water molecules can form aggregates with ice-like structure. Heterogeneous nucleation is thought to occur both indirectly through the liquid phase as well as directly from the gas to the ice phase. Heterogeneous freezing, that is heterogeneous nucleation from the liquid phase, occurs when a cloud droplet or a solution droplet comes in contact with an INP upon which the droplet freezes. Heterogeneous freezing may also occur when water vapor condenses directly onto the INP followed by freezing of the liquid nucleus formed on the INP.

Alternatively, heterogeneous nucleation may occur directly from the vapor phase by deposition of water molecules directly onto the INP. It is, however, still debated whether this process really occurs directly from the vapor phase or whether an intermediate liquid nucleus is formed on the INP.

2.3.2 Growth processes

In principle, the growth processes for ice particles are the same as for liquid droplets. However, due the potential coexistence of particles in the liquid phase these processes have slightly different characteristics as will be explained below.

Due to the lower saturation vapor pressure of ice compared to that of water, a newly-formed ice nucleus experiences a much higher ratio of supersaturation then a cloud droplet would. Because of this, the diffusional growth of ice crystals is much faster than that for cloud droplets. The rapid growth of the ice particles will deplete the surrounding air of water vapor. This depletion may cause the environment to become sub-saturated with respect to water but saturated with respect to ice. If this is the case, potentially present supercooled cloud droplets evaporate and their molecules deposit onto the ice particles. This is known as the Wegener-Bergeron-Findeisen process.

Similar as for cloud droplets, an ice crystal that grows sufficiently in mass eventually starts to sediment. Size differences between different particles as well as turbulence may cause particles to collide and potentially stick together to form larger particles thus initiating growth by accretion. Accretion is the general term for the growth of two hydrometeors caused by a collision and resulting in permanent union of the two particles. For ice particles growth by accretion can happen in two ways: The collision of two ice particles, called aggregation, or the collision of an ice particle with a liquid particle which freezes upon contact, called riming. Aggregation produces aggregates of snow crystals that, if they don't melt, fall to the ground in the form of snow. Particles produced by riming a known as graupel, when their diameter remains below 2.5 mm, and hail for sizes above that.

2.3.3 Ice habits

Ice crystals exhibit a fascinating range of different forms. Their crystal structure depends on the thermodynamic conditions of their formation. This is due to the dependence of the surface tension on the temperature and supersaturation as well as the tendency of the shape to minimize this surface tension.

A common grouping of ice particles is into pristine ice crystals, aggregates and rimed particles. Common shapes for ice crystals are plates and columns. But also other shapes such as dendrites, stellar plates or needles can be observed. Snow aggregates are usually made up of 10 to 100 or more single crystals. They often consist of dendrites and thins plates. Finally, rimed particles are typically spherical with densities slightly lower than that of solid ice due air inclusions.

2.4 Precipitation

Chapter 3

Microwave radiative transfer in the atmosphere

The underlying physical mechanism that allows cloud and precipitation to be remotely sensed is their interaction with electromagnetic radiation that can be measured from afar using suitable detectors. These interactions are described by the theory of radiative transfer. Since this theory is essential for the understanding and development of retrieval methods, this section provides an introduction to the radiative transfer of microwaves in the atmosphere. Particular focus is put on the interaction of radiation with clouds. This presentation is mostly based on the more comprehensive texts by Thomas and Stamnes (2002), Mishchenko et al. (2002), and Wallace and Hobbs (2006).

3.1 The theory of radiative transfer

Radiative transfer theory describes radiation as monochromatic beams that transport radiant energy through the atmosphere. One of the fundamental quantities of the theory is the spectral intensity I_ν defined as the rate at which a beam of angular extent $d\omega$ propagating into direction $\hat{\boldsymbol{n}}$ of frequency ν transports energy through an infinitesimal area dA:

$$I_\nu = \frac{d^5 E}{\cos(\theta) dA \; dt \; d\omega \; d\nu} \tag{3.1}$$

In addition to that, a monochromatic beam of radiation has a polarization state, which describes how the energy flux is split up between the two components of the electric field perpendicular to the propagation direction as well as their respective phase. The intensity of a beam and its polarization state are described by the stokes vector

$$\boldsymbol{I} = \begin{bmatrix} I_\nu \\ D \\ Q \\ U \end{bmatrix} \tag{3.2}$$

The four components I, D, Q and U of the Stokes vector fully characterize an electromagnetic plane wave to the extent it that it can be measured using traditional detectors. This means that all its measurable quantities can be derived from the corresponding stokes vector.

The stokes vector can be directly related to the electromagnetic field strength of an electromagnetic plane wave allowing it to be derived from the more fundamental theory of electromagnetism. The key advantage of radiative transfer theory, however, is that it allows a simplified treatment of the problems relevant to atmospheric remote sensing which are too complex to be solved by direct application of the laws of electrodynamics.

3.1.1 Interactions with matter

The Stokes vector provides a full description of the radiation measured by any remote sensing instrument. To model the radiation reaching the detector, a suitable description how this radiation is created as well as how it changes as it propagates through the atmosphere is required. A common approach in radiative transfer theory is to distinguish three fundamental types of such interactions of radiation with matter: The emission of radiation, its absorption, and the scattering of absorption away from its propagation path.

Emission

At temperatures above absolute zero, all matter emits radiation through the process of thermal emission. Thermal emission occurs when matter transitions from a quantum mechanical state of higher energy to one of lower energy which causes the surplus of energy to be emitted in the form of radiation. When considering radiation in the lower atmosphere, the relevant emitters of radiation are the ocean or land surface as well as gas molecules or suspended particles.

A fundamental concept for the description of emission is that of a black body. A black body is a piece of matter that absorbs all incoming radiation. At a given temperature T, the emission of a black body is isotropic and polarized. Its spectral intensity is given by Planck's law:

$$B_\nu(\nu, T) = \frac{2h\nu^3}{c^2}\frac{1}{\exp(\frac{h\nu}{k_BT}) - 1} \tag{3.3}$$

where c is the speed of light in the medium, h is the Planck constant and k_B is the Boltzmann constant. The stokes vector describing the emission from a black body is given by

$$\boldsymbol{I} = \begin{bmatrix} B_\nu \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{3.4}$$

The concept of the black body is used to define the emission from other forms of matter using the emissivity vector $\boldsymbol{\epsilon}$:

$$\boldsymbol{I} = \boldsymbol{\epsilon} \cdot B_\nu \tag{3.5}$$

The main difference between the treatment of emission from a volume compared to that of a surface is the unit of the emission vector $\boldsymbol{\epsilon}$. For a volume, it is defined per unit length of the path through the volume, while for a surface this is not necessary.

Due to the distinct orientation that surfaces have with respect to the viewing geometry, the emissivity vector generally depends on the incidence angle. For particles this is generally also the case, but since most particles in the atmosphere are randomly oriented it is often neglected. Although black-body radiation is unpolarized, emission from general emitters can be polarized. An important example is the ocean surface, which is highly polarized around the Brewster angle at 53°.

Absorption

Absorption refers to the process of radiation being converted into internal energy of the matter it interacts with. Mathematically, absorption is described by an absorption vector $\boldsymbol{\alpha}$, defined as the fraction of the incoming radiation that is absorbed along an infinitesimal distance ds along the propagation path:

$$\boldsymbol{I}_{\text{absorbed}} = (\boldsymbol{\alpha} \cdot \; ds) \odot \boldsymbol{I} \tag{3.6}$$

Here $\odot$ denotes the element-wise product of the absorption vector and the stokes vector $\boldsymbol{I}$ of the incoming radiation. Absorption may be understood as the inverse process of thermal emission. Formally, this is expressed by Kirhoff's law of radiation

$$\boldsymbol{\alpha} = \boldsymbol{\epsilon} \tag{3.7}$$

This law is applicable to all matter in the atmosphere given that it is in a state of local thermal equilibrium (LTE). LTE occurs when the density of matter is sufficiently high so that the population frequencies of energy states above the ground state are determined by thermal collisions rather than the absorption of radiation. This decouples the emission of radiation from the radiation field, allowing the simplified treatment of matter as thermal emitters with the emission rates independent of the radiation field. LTE is a valid assumption for radiative transfer in the lower atmosphere.

Scattering

When a beam of radiation impinges upon a particle, their interaction may cause a deviation of parts of the beam from the original propagation path. To first order, scattering decreases the intensity of the beam. This particular process is referred to as single scattering. As it propagates through the atmosphere, the intensity of a beam is decreased by the effects of absorption and single scattering. The combination of these two processes is referred to as attenuation.

However, as the rate of scattering increases, also the effect of multiple scattering has to be taken into account. Multiple scattering occurs when energy from other beams scattered into the line of sight causes an increase in the intensity of the considered beam.

Mathematically, the scattering of a beam of light propagating in direction $\boldsymbol{n}$ into the direction $\hat{\boldsymbol{n}}$ is described by the phase matrix $\boldsymbol{Z}(\boldsymbol{n}, \hat{\boldsymbol{n}})$:

$$\boldsymbol{I}_{\text{scattered}}(\hat{\boldsymbol{n}}) = \boldsymbol{Z}(\hat{\boldsymbol{n}}, \boldsymbol{n})\boldsymbol{I}(\boldsymbol{n}) \tag{3.8}$$

The combined, attenuating effects of scattering and absorption are give by the attenuation matrix $\boldsymbol{K}$, given by the sum of the absorption vector $\boldsymbol{a}$ and the fraction of radiation scattered away from the propagation path:

$$\boldsymbol{K} = \boldsymbol{\alpha} + \int_{\hat{\boldsymbol{n}}} d\hat{\boldsymbol{n}}\ \boldsymbol{Z}(\hat{\boldsymbol{n}}, \boldsymbol{n}) \tag{3.9}$$

3.1.2 The radiative transfer equation

The previous section introduced the fundamental interactions of radiation with matter and how they are described mathematically in radiative transfer theory. Combining the three processes of emission, absorption and scattering, the change that a beam undergoes as it travels a distance ds along its propagation path through the atmosphere is described the vectorized radiative transfer equation (VRTE):

$$\frac{d\boldsymbol{I}}{ds} = -\boldsymbol{K}\boldsymbol{I} + \boldsymbol{\alpha} \cdot B_\nu(T) + \int_\Omega d\omega\ \mathbf{Z}(\boldsymbol{n}, \hat{\boldsymbol{n}})I(\hat{\boldsymbol{n}}). \tag{3.10}$$

By solving Equation (3.10) the radiation field for an arbitrary atmosphere can be computed. What is required for this are the values of temperature, absorption vector $\boldsymbol{\alpha}$ and phase matrices $\boldsymbol{Z}$ throughout the atmosphere as well as a suitable method for solving the radiative transfer equation. The values of $\boldsymbol{\alpha}$ and $\boldsymbol{Z}$ describe how a specific volume element of the atmosphere absorbs and scatters radiation. Their values therefore depend on the concentrations of gases and particulate matter in the atmosphere.

Approximate values of $\boldsymbol{\alpha}$ and $\boldsymbol{Z}$ for different materials in the atmosphere can be measured experimentally or in special cases even derived from first principles. Typically they depend on local properties of the atmosphere such as temperature, pressure or concentration of gases or particles. Numerical models for $\boldsymbol{\alpha}$ and $\boldsymbol{Z}$ together with the VRTE thus allow the radiation field observed by remote sensing intruments to be related to the state of the atmosphere. Together with the methods described in Section 4, this forms the basis of atmospheric remote sensing.

3.1.3 Long-wave radiative transfer in the atmosphere

This thesis focuses on observations of the atmosphere at microwave and sub-millimeter wavelengths. The specific properties of this frequency domain allow for a number of simplifications, that can greatly simplify the solution of the VRTE in the atmosphere.

At microwave frequencies, all relevant emission of radiation is due to thermal emission from matter in the atmosphere. Emission from the sun is irrelevant at these wavelengths. Furthermore, due to the long wavelengths of the radiation, scattering by molecules of gases can be neglected. In this case, the integral in Eq. (3.10) disappears and it can be solved efficiently by integration along the line of sight.

In the presence of clouds, solving the radiative transfer equation becomes more complicated and computationally more demanding as it requires solving for the whole radiation field instead of solving the VRTE along a single beam.

3.2 Microwave observations of clouds and precipitation

Clouds and precipitation can be observed at microwave frequencies using active as well as passive observation techniques.

3.2.1 Radar observations

3.2.2 Passive observations

Chapter 4

Inverse problems

The previous chapter introduced the general properties of clouds and their effect on electromagnetic radiation which can be used to observe them. This chapter describes the mathematical methods that can be used infer properties of clouds from their signatures in the observed electromagnetic radiation. Mathematically, this problem can be formulated as an inverse problem. This is because inferring the cloud properties from the observations may be viewed as the inverse of the problem of predicting the observations from the cloud properties, which can be solved using radiative transfer. This, the problem of solving the radiative transfer equation in the presence of cloud hydrometeors, is referred to as the forward problem.

4.1 Formulation

Mathematically, the inverse problem is formulated as follows: Let $\boldsymbol{x} \in \mathbb{R}^n$ be an arbitrary vector from the state space $\mathbb{R}^n$. Here it is assumed that the vector $\boldsymbol{x}$ describes the properties of the observed cloud. The space $\mathbb{R}^n$ is the space of all possible cloud configurations that could be observed. The interaction of the cloud described by the vector $\boldsymbol{x}$ interacts with the radiation that is measured by an observation system, producing the observation vector $\boldsymbol{y}$. It is assumed here that a so called forward $\mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ exists that allows computing the observation $\mathbf{F}(\boldsymbol{x})$ corresponding to any given state vector $\boldsymbol{x}$. The inverse problem now consists of determining the state vector $\boldsymbol{x}$ corresponding to a given observation $\boldsymbol{y}$ thus inverting the forward model $\mathbf{F}$.

The general difficulty with inverse problems is that they do not admit a unique solution. This is because, at least in atmospheric remote sensing, the problem is generally underconstrained. This means that the amount of information in the observations $\mathbf{y}$ is not sufficient to uniquely determine a state $\mathbf{x}$. Examples are different cloud configurations that result in the same measurement vector such as for example a low-level cloud covered by an opaque high-level cloud. From the measurement vector $\boldsymbol{y}$ alone it is impossible to determine a unique state $\boldsymbol{x}$ as it will be the same independent of the presence of properties of the low-level cloud.

Simultaneously to being underconstrained, the problem may be over constrained. This happens if different components of the measurement vector provide seemingly contradictory information on the measurement state $\boldsymbol{x}$ due errors random errors in $\boldsymbol{y}$.

4.2 Solution

A common approach in atmospheric remote sensing to solving inverse problems is the application of Bayesian statistics. Instead of searching a unique solution vector $\boldsymbol{x}$ to the inverse problem, the solution is found in the form of a probability distribution that describes how likely it is that any of the elements of the state space have produced the given observation $\boldsymbol{y}$.

The approach that will be presented in the following is known as the optimal estimation method (OEM, Rodgers (2000)). The method makes three basic assumptions in order to solve the inverse problem:

1. That the forward model $\mathbf{F}$ is linear or only weakly non-linear
2. That the knowledge available about $\boldsymbol{x}$ can be described by a Gaussian distribution with mean $\boldsymbol{x}_a$ and covariance matrix $\boldsymbol{S}_a^{-1}$
3. That the errors affecting $\mathbf{y}$ are Gaussian with covariance matrix $\boldsymbol{S}_\epsilon$

Under these assumption both the a priori distribution for $\boldsymbol{x}$ as well as the conditional probability of observing the measurement $\boldsymbol{y}$ given the state $\boldsymbol{x}$ are Gaussian:

$$p(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{-n}{2}}\det(\boldsymbol{S}_a)^{-\frac{1}{2}}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_a)^T\boldsymbol{S}_a^{-1}(\boldsymbol{x}-\boldsymbol{x}_a)\right\} \tag{4.1}$$

$$p(\boldsymbol{y}|\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{-m}{2}}\det(\boldsymbol{S}_e)^{-\frac{1}{2}}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\mathbf{F}(\boldsymbol{x}))^T\boldsymbol{S}_e^{-1}(\boldsymbol{x}-\mathbf{F}(x))\right\} \tag{4.2}$$

In the Bayesian framework the solution of the inverse problem is simply the a posteriori distribution $p(\boldsymbol{y}|\boldsymbol{x})$ of $\boldsymbol{x}$ given the observation vector $\boldsymbol{y}$. It is found by applying Bayes theorem

$$p(\boldsymbol{y}|\boldsymbol{x}) = \frac{p(\boldsymbol{y}|\boldsymbol{x})p(\boldsymbol{x})}{p(\mathbf{y})} \tag{4.3}$$

$$\propto p(\boldsymbol{y}|\boldsymbol{x})p(\boldsymbol{x}) \tag{4.4}$$

to the probabilities (4.1) and (4.2).

As a specific solution of the retrieval problem, generally the most likely state is chosen, denoted as the maximum a posteriori (MAP) estimator for $\boldsymbol{x}$. It can be found by minimizing the log-likelihood of the posterior distribution, which has the form:

$$-\mathcal{L} \propto (\boldsymbol{F}(\boldsymbol{x})-\boldsymbol{y})^T\boldsymbol{S}_\epsilon^{-1}(\boldsymbol{F}(\boldsymbol{x})-\boldsymbol{y})(\boldsymbol{x}-\boldsymbol{x}_a)^T\boldsymbol{S}_a^{-1}(\boldsymbol{x}-\boldsymbol{x}_a) \tag{4.5}$$

Solving the retrieval problem has thus been reduced to minimizing the negative log likelihood of the posterior distribution. When the forward model is non-linear, minimizing (4.5) must be performed iteratively using suitable optimization methods such as the Gauss-Newton or Levenberg-Marquardt methods (Boyd and Vandenberghe 2004).

4.3 Error estimation

When the forward model is approximately linear around the retrieved state $\boldsymbol{x}$, the covariance of the a posteriori distribution is given by

$$\mathbf{S} = \left(\boldsymbol{K}^T \boldsymbol{S_\epsilon}^{-1} \boldsymbol{K} + \boldsymbol{S}_a^{-1}\right)^{-1}. \tag{4.6}$$

Here $\boldsymbol{K}$ is the Jacobian of the forward model evaluated at the retrieved state $\boldsymbol{x}$.

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