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Studies of Atmospheric Dynamics from Space

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de Rector Magnificus, prof.dr.ir. C.J. van Duijn, voor een commissie aangewezen door het College voor Promoties in het openbaar te verdedigen op woensdag 6 april 2005 om 16:00 uur

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Samenvatting

De lucht in de atmosfeer van de aarde is voortdurend in beweging. Deze bewegingen worden opgewekt en beïnvloed door een groot aantal factoren, zoals opwarming en afkoeling, de draaiing van de aarde en obstakels waar de lucht omheen moet. Een goed begrip van alle bewegingen (dynamische processen) die plaatsvinden in de atmosfeer is belangrijk omdat deze processen een rol kunnen spelen bij bv. klimaatveranderingen en de afbraak en het herstel van de ozonlaag. Door middel van atmosferische computermodellen en metingen aan de eigenschappen van de atmosfeer proberen wetenschappers een zo compleet mogelijk beeld te krijgen van de processen, zowel chemisch als dynamisch, die de toestand van de atmosfeer beïnvloeden.

Metingen aan de atmosfeer zijn er in vele soorten die o.a. verschillen in de locatie waar het instrument is opgesteld. Zo kunnen metingen uitgevoerd worden vanaf de grond, maar ook vanaf vliegtuigen, ballonnen, schepen of satellieten. Daarnaast kunnen de metingen informatie verschaffen over ofwel de toestand van de atmosfeer op de locatie van het instrument zelf ofwel vanaf een afstand een deel van de atmosfeer waarnemen. In het tweede geval wordt er straling (bv. afkomstig van de zon) gemeten die informatie bevat over het deel van de atmosfeer waar de straling doorheen gegaan is.

Veel metingen hebben slechts een beperkte geografische dekking en geven hierdoor een onvolledig beeld van de dynamische processen die plaats hebben in de atmosfeer. Vooral grootschalige processen worden dan niet goed omvat. Echter, satelliet instrumenten die rond de aarde cirkelen, kunnen metingen uitvoeren die een groot deel, zo niet de gehele aarde beslaan. Om deze reden vormen satellietmetingen een uniek middel voor het op mondiale schaal bestuderen van dynamische en chemische processen in de atmosfeer.

De titel van dit proefschrift luidt vertaald: 'Studies van dynamische processen in de atmosfeer vanuit de ruimte' en richt zich op twee verschillende fenomenen: Equatoriale Kelvin golven en daling in de polaire vortices. Wat deze fenomenen precies inhouden zal hieronder beschreven worden. Voor de bestudering van de processen wordt gebruik gemaakt van satellietmetingen van respectievelijk het Global Ozone Monitoring Experiment (GOME) en het Improved Limb Atmospheric Spectrometer (ILAS) instrument.
### Equatoriale Kelvin golven

Golven in de atmosfeer zijn zichtbaar als oscillaties in ondermeer snelheden van luchtstromingen, luchtdruk en temperatuur, die zich voortplanten in de atmosfeer. Equatoriale Kelvin golven zijn golven in de atmosfeer die alleen voorkomen in de tropen. Deze golven bewegen van west naar oost, en hebben in de meeste gevallen een lengte gelijk aan de omtrek van de aarde (golfgetal 1) of de helft hiervan (golfgetal 2).

![Schematische illustratie van golfgetal 1 en 2.](image)

Een Kelvin golf met golfgetal 1 zal dus een positieve luchtdruk verstoring veroorzaken aan de ene kant van de aarde en tegelijkertijd een negatieve luchtdruk verstoring aan de andere kant. Deze verstoringen planten zich naar het oosten voort en hebben een verticale golflengte van ongeveer 10 km. Kelvin golven worden aangeslagen door grootschalige opwarming en opstijging van lucht in de tropen. De golven planten zich ook omhoog voort totdat ze een hoogte bereiken waar de condities zo zijn dat de golven breken of reflecteren. De energie en oostwaartse impuls (hoeveelheid van beweging) die de golven bezitten wordt bij breking overgedragen aan de achtergrondstroming. Deze overdracht van energie en impuls beïnvloed de snelheid en richting van de achtergrondstroming en speelt een rol in de aandrijving van belangrijke windschommelingen in de tropische atmosfeer. Zo bestaat er een ongeveer tweejaarlijkse windschommeling, de quasi-biennial oscillation (QBO), die zichtbaar is in de gemiddelde zonale (oost-west of west-oost) wind in de tropische atmosfeer tussen ongeveer 15 en 35 km hoogte. De wind verandert op deze hoogte dus van oostenwind naar westenwind en andersom met een periode van ongeveer 2 jaar. De QBO is een belangrijk proces dat o.a. invloed heeft op orkaanactiviteit, tropische cyclonen, regenvalpatronen en transport van vulkanisch stof na een uitbarsting. Het is dus belangrijk om de QBO goed te kunnen beschrijven en voorspellen met modellen en daarvoor is informatie nodig over de aandrijving van de QBO. In welke mate Kelvin golven een rol spelen bij deze aandrijving is nog niet goed bekend. Voor het onderzoeken hiervan zijn metingen van Kelvin golfactiviteit cruciaal.

Zoals eerder gezegd zijn Kelvin golven zichtbaar als oscillaties in zonale (oost-west of west-oost) en verticale snelheden en temperatuur (door de stijging en daling en daardoor uitzetting en samendrukking van lucht). Daarnaast kunnen de golven
Samenvatting

verstoringen in concentraties van sporengassen\(^1\) in de atmosfeer veroorzaken, hetzij door de snelheidssfluctuaties, i.e. transport, hetzij door de temperatuur fluctuaties via de temperatuursafhankelijkheid van chemische reacties die het sporengas produceren of afbreken (fotochemische effecten). Metingen van bv. ozon kunnen dus fluctuaties vertonen die in verband kunnen worden gebracht met equatoriale Kelvin golven.

**Daling in de polaire vortices**

De hoeveelheid zonnestraling die de aarde bereikt is groter bij de evenaar dan bij de polen. De atmosfeer wordt hierdoor meer opgewarmd bij de evenaar en er ontstaat een temperatuurs- en luchtdrukverschil tussen de evenaar en de polen. Door het drukverschil zal er lucht van de evenaar (hoge druk) naar de polen bewegen (lage druk) en door de draaiing van de aarde buigt de lucht ten opzichte van het aardoppervlak af en zal in oostwaartse richting bewegen. Het afbuigeffect is groter bij de polen en zorgt ervoor dat de windsnelheid (van west naar oost) groter is dichter bij de polen. Dit hele proces veroorzaakt een wervelachtige kronkelende stroming rond de polen die de polaire jet wordt genoemd (zie onderstaand figuur).

Schematische illustratie van het ontstaan van de polaire jet, de vortex en de gemiddelde grootschalige circulatie in noord zuid richting op het noordelijk halfrond. H staat voor hoge druk en L voor lage druk.

In de winter van elk halfrond (december-februari op het noordelijk halfrond en juni-augustus op het zuidelijk halfrond) wordt het temperatuursverschil tussen evenaar en polen groter en de polaire jet sterker. Het gebied gecentreerd rond de pool dat begrensd wordt door de polaire jet wordt de polaire vortex genoemd. De polaire vortex is dus een gebied rond de pool met koude lucht dat afgebakend wordt door een sterke stroming. Wanneer deze stroming sterk genoeg is, zal de lucht van binnen de vortex afgesloten zijn van de lucht erbuiten en vindt er geen menging plaats tussen beide luchtmassa’s.

De gemiddelde grootschalige circulatie in noord-zuid (en zuid-noord) richting in de atmosfeer wordt gekarakteriseerd door opwaartse beweging in de tropen, poolwaartse

\(^1\)Sporengassen zijn de gassen die zich in zeer geringe hoeveelheden in de atmosfeer bevinden naast zuurstof, stikstof en argon. Voorbeelden zijn ozon, stikstofoxide, koolstofdioxide, en waterdamp.
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stroming op het winter halfrond en neerwaartse beweging op hoge breedtegraden (zie bovenstaand figuur). In de polaire vortices vindt dus neerwaartse beweging plaats.

De concentratie van sporengassen in de atmosfeer, die een lange levensduur hebben en dus niet snel worden afgebroken in de atmosfeer, verandert weinig binnen een luchtmassa die bewegingen ondergaat. Door het volgen van een constante concentratie van een sporengas kan dus informatie gewonnen worden over de luchtbewegingen zoals de daling in de polaire vortices. In dit proefschrift zullen constante concentraties van het sporengas N\textsubscript{2}O (distikstofmonoxide ofwel lachgas) gevolgd worden om de daling binnen de polaire vortices te bepalen. Deze waardes zijn o.a. nodig bij berekeningen waarbij de banen van luchtmassa’s terug of vooruit in de tijd bepaald worden, zogenaamde trajectoriën.

GOME

Het GOME instrument is op 21 april 1995 gelanceerd aan boord van de ERS-2 (second European Remote Sensing) satelliet. Het belangrijkste doel van het instrument is het bepalen van de concentraties van sporengassen die een rol spelen in de ozon chemie. GOME meet de zonnestraling die door de atmosfeer terug de ruimte in wordt verstrooid of die door het aardoppervlak wordt gereflecteerd. Dit noemen we de aard-radiantie. Daarnaast wordt de zonne-radiantie die direct van de zon komt gemeten, de zogenaamde zonne-irradiantie. De verhouding tussen de aard-radiantie en zonne-irradiantie wordt bepaald door de processen in de atmosfeer die de straling beïnvloeden, zoals absorptie door gassen en verstrooiing door luchtmoleculen en stofdeeltjes. De absorptie door elk sporengas is verschillend in sterkte en is afhankelijk van de golflengte van de straling. Ozon bijvoorbeeld absorbeert heel sterk bij golflengtes tussen de 200 en 350 nm. Met behulp van een fysisch model dat gebruik maakt van ondermeer de absorptie karakteristieken van elk sporengas wordt bepaald hoe de metingen verwacht worden eruit te zien bij verschillende concentraties van de sporengassen. Door vervolgens de uitkomsten van het model zo goed mogelijk te laten overeenkomen met de gemeten waardes kan bepaald worden welke concentraties leiden tot de gemeten waardes. Dit proces wordt retrieval genoemd. In dit proefschrift worden totale ozon kolommen (de hoeveelheid ozon in een verticale kolom) en verticale ozon profielen (ozon op verschillende hoogtes) van GOME gebruikt.

ILAS

ILAS is een satellietinstrument dat zich aan boord van de satelliet ADEOS (Advanced Earth Observing Satellite) bevond. Het instrument heeft 8 maanden aan data verkregen van 1 November 1996 tot 30 Juni 1997, toen een defect zonnepaneel het einde van de ADEOS missie betekende. ILAS gebruikte een occultatie techniek waarbij bij zonsopkomst en zonsondergang naar de zon gekeken wordt en de zonne-radiantie gemeten wordt die door de atmosfeer heen het instrument bereikt (figuur 1.7). Wederom worden de karakteristieke absorptie eigenschappen van de sporengassen gebruikt om hun concentraties af te leiden. Omdat het instrument meet bij zonsopgang en zonsondergang, gezien vanuit het instrument, is de geografische bedekking beperkt tot de gebieden rond de polen tot maximaal zo’n 55° op het noordelijk halfrond of 65° op
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het zuidelijk halfrond (figuur 1.8). Een van de sporengassen die gemeten wordt is N\textsubscript{2}O (distikstofmonoxide of lachgas).

Dit proefschrift

Het grootste deel van dit proefschrift (hoofdstuk 3 tot en met hoofdstuk 5) gaat over de detectie en analyse van Kelvin golven in de ozon metingen van GOME. De GOME ozon kolommen (hoofdstuk 3) en profielen (hoofdstuk 5) worden geanalyseerd met behulp van een tweedimensionale spectrale methode (in tijd en zonale richting) die Lomb periodogram genoemd wordt. De methode berekent welke golffrequencies dominant zijn in een 60-daagse periode. Een groot voordeel van de methode is de directe bepaling van de significantie van de gedetecteerde signalen.

In 7 jaar GOME ozon kolom data zijn drie 60-daagse periodes met hoge Kelvin golf activiteit waargenomen die samenvallen met equatoriale oostenwinden op het drukniveau van 30 hPa (~25 km hoogte): 15 juli tot 13 september 1996, 17 juli tot 15 september 1998 en 19 september tot 18 november 2000. De correlatie tussen de hoge Kelvin golf activiteit en de oostenwinden is in overeenkomst met de theorie dat de Kelvin golven niet door westenwinden heen kunnen propageren. In de drie genoemde periodes vinden we oostwaartse golven met zonaal golfgetal 1 en 2 en periodes van 12 tot 15 dagen. De door de Kelvin golven veroorzaakte fluctuaties in de ozon kolommen bedragen 1 tot 2 Dobson Unit (DU)\textsuperscript{2} en kunnen toegeschreven worden aan langzame Kelvin golven in de lagere stratosfeer\textsuperscript{3}.

Twee verschillende datasets van GOME ozon profielen zijn geanalyseerd, OPERA en NNORSY, die verschillen in de methode die gebruikt is om uit de stralingsmetingen ozonconcentraties te berekenen. Daarnaast is een derde set geanalyseerd die bestaat uit de OPERA ozon profielen gecombineerd met een 3D chemie-transport model (geassimuleerde ozon profielen).

Alle drie de datasets vertonen Kelvin golf signalen die overeenkomen met de signalen in de ozon kolommen voor de drie periodes met hoge Kelvin golf activiteit. De eerste twee sets kunnen echter niet volledig de verticale structuur van de Kelvin golven oplossen. Dit wordt veroorzaakt door een te laag oplossend vermogen in de hoogte, fijne verticale structuren worden niet opgelost. De derde set met geassimuleerde profielen geeft meer hoogte informatie over de Kelvin golf activiteit die overeenkomt met resultaten van andere studies. Deze informatie is waarschijnlijk afkomstig van de meteorologische velden (wind en temperatuur) van het ECMWF (European Centre for Medium-range Weather Forecast) die in het model worden gebruikt.

Maximale Kelvin golf verstoringen zijn zichtbaar op een drukniveau van 35 hPa, de hoogte waar de verticale gradient in ozon het grootst is. Dit is volgens verwachting wanneer alleen transport effecten meegeno men worden en fotochemische effecten worden verwaarloosd. Verder vinden we grote fluctuaties in de ozon mengverhouding op hoogtes tussen de 10 en 1 hPa. Echter de ozonconcentratie op deze hoogte is laag zodat deze fluctuaties geen grote bijdrage leveren aan de fluctuaties in de totale ozon

\textsuperscript{2}100 DU komt overeen met een ozonlaag van 1 mm als alle ozon zich in een verticale kolom met een druk van 1013.25 hPa (standaard gronddruk) en 0\textdegree C bevindt.

\textsuperscript{3}De stratosfeer is de laag in de atmosfeer die zich in de tropen uitstrekt van ongeveer 15 km tot 50 km hoogte (zie figuur 1.1)
hoeveelheid in een kolom. Sommering van de fluctuaties op alle hoogtes geeft ozon kolom fluctuaties van 1 à 2 DU overeenstemmend met de waardes gevonden bij de analyse van de ozon kolommen.

In hoofdstuk 4 bestuderen we de Kelvin golf signalen in de ECMWF Re-Analysis (ERA-40) wind en temperatuurvelden. Deze dataset is geproduceerd door de combinatie van meteorologische waarnemingen met een mondiaal weermodel. Voor de drie periodes waarin we hoge Kelvin golf activiteit vonden in de GOME ozon kolommen vertoont de ERA-40 data overeenkomende signalen. De signalen zijn zichtbaar tussen de 100 en 10 hPa. De maximale door Kelvin golven veroorzaakte fluctuaties in zonale wind en temperatuur zijn respectievelijk 8 m/s en 2K. Wanneer we alleen rekening houden met transport effecten dan kunnen deze fluctuaties volgens de theorie leiden tot totale ozon kolom fluctuaties van ongeveer 1 DU. De maximale ozon fluctuaties rond 35 hPa in de geassimuleerde ozon profielen lopen in fase met ERA-40 temperatuur fluctuaties, dit is een indicatie dat de ozon fluctuaties op deze hoogte voornamelijk worden veroorzaakt door transport effecten. De fluctuaties in ozon mengverhouding die zichtbaar zijn tussen de 10 en 0.1 hPa, lopen in tegen fase met de temperatuur fluctuaties. Dit kan veroorzaakt zijn door zowel transport als fotochemische effecten. Verder onderzoek is nodig om te herleiden hoe groot de bijdrages van beide componenten zijn aan deze ozon fluctuaties.

Hoofdstuk 6 richt zich op het bepalen van de daling en stijging binnen (en buiten) de polaire vortices.Hiervoor worden constante waardes van N\textsubscript{2}O concentraties getraceerd. Op het zuidelijk halfrond vinden we voorafgaand aan de vorming van de polaire vortex sterke daling. Na de vorming van de polaire vortex duurt de daling binnen de vortex voort. De gevonden waardes komen overeen met andere studies. Op het noordelijk halfrond omvat de meetperiode niet de periode voorafgaand aan de vorming van de vortex. Daling is zichtbaar binnen de vortex op hoogtes onder de potentiele temperatuur\textsuperscript{4} niveaus van 700-800 K. De berekende waardes zijn hier lager dan op het zuidelijk halfrond en liggen binnen het bereik van berekende waardes in andere studies. Na het opbreken van de polaire vortex is stijging zichtbaar.

Samenvattend demonstreert dit proefschrift het vermogen van satellietmetingen om op een mondiale schaal het inzicht in enkele belangrijke dynamische processen in de atmosfeer te vergroten en beter te beschrijven.

\textsuperscript{4}De potentiele temperatuur is de temperatuur die een luchtmassa zou hebben als die zonder warmte uitwisseling met de omgeving wordt gebracht naar een standaarddruk (meestal de grond- druk). Op het aardoppervlak is de potentiele temperatuur dus gelijk aan de gewone temperatuur. De potentiele temperatuur van een luchtmassa kan alleen maar veranderen als er warmte wordt toe- of afgevoerd.
Introduction

The state of the Earth’s atmosphere is continuously influenced by both dynamical and chemical processes. Many of these processes are not fully understood yet. To improve the understanding and description of the processes taking place in the atmosphere, use is made of atmospheric computer models, process studies and measurements. These measurements differ in measurement method (instrument type) and instrument platform. The most common platforms are the ground, aircraft, balloon, ship and satellites. The instruments can either provide information on the state of the atmosphere at the location of the instrument or remotely sense a part of the atmosphere e.g. by measuring radiation containing information on the part of the atmosphere it passed through. Because of their restricted geographical coverage, most measurements only provide a picture of part of the processes taking place. Especially large scale processes are not well captured. Satellites circling around the Earth can however take measurements covering the entire or a large part of the globe. Therefore satellite measurements provide a unique mean to study dynamical and chemical processes on a global scale.

In this thesis two different phenomena are studied using satellite measurements: Equatorial Kelvin waves with the Global Ozone Monitoring Experiment (GOME) instrument and diabatic descent in the polar vortices using Improved Limb Atmospheric Spectrometer (ILAS) measurements.

This first chapter will give a short introduction on the vertical structure of the atmosphere, equatorial Kelvin waves, subsidence in the polar vortices and satellite measurements.

1.1 Structure of the atmosphere

Depending on composition and dominance of physical processes the Earth’s atmosphere can be divided into different layers (see Figure 1.1). The lowest layer is called the troposphere. The troposphere extends from the surface of the Earth up to the tropopause, which is situated at a height of approximately 8 km in polar regions and 16 km in the tropics (see Figure 1.2).

In the troposphere the temperature decreases with height. The layer above the tropopause is called the stratosphere. The stratosphere extends up to the stratopause at around 50 km height. In this layer the temperature increases with height.
Both the composition and the dynamical processes taking place are different in the troposphere and stratosphere. For example, most of the water vapor in the atmosphere can be found in the troposphere, especially in the lower troposphere. In the stratosphere the amount of water vapor is very low. In the troposphere the large scale vertical mixing of air is rapid (in the order of days), whilst in the stratosphere the mixing takes place on longer timescales (in the order of months). The reason for this is the difference in temperature gradient in both layers. In the troposphere
there is warm air below colder air, often leading to an unstable situation where e.g. convection takes care of rapid vertical mixing. In the stratosphere the temperature increases with height, which is a stable situation. Because of this temperature structure, the tropopause forms a barrier between the troposphere and stratosphere. The exchange of air between both layers is small but very important for the atmospheric composition and subject of many studies.

The layer above the stratopause is called the mesosphere. The temperature in this layer decreases with height up to the mesopause (at 80-90 km), which is primarily because of the decrease of ozone with height and corresponding reduction of absorption of solar radiation. Above the mesosphere we find the thermosphere where the temperature increases rapidly with height because of the ionisation of oxygen and nitrogen. This thesis focuses on processes taking place mainly in the stratosphere.

1.2 Equatorial Kelvin waves

In the tropics the incoming radiation flux from the sun causes strong heating of the Earth’s surface. Thereupon the air close to the surface heats up and rises. When this rising of air, called convection, takes place on large scales it can lift air up to the tropopause and generate different types of waves. One of these wave types is the Kelvin wave. It is named like this because of its similarity with the coastal trapped oceanic Kelvin wave, which was discovered by Lord Kelvin in 1879. The atmospheric Kelvin wave is a wave type that only exists in the equatorial region. The force balance governing this wave type is controlled by the stratification of the air and the change of sign of the Coriolis force at the equator. It is an eastward moving wave, without latitudinal component, observed mostly with wavelengths equal to the circumference of the Earth or half of it, i.e. zonal wavenumbers 1 or 2. The waves propagate vertically, with an amplitude increasing exponentially with height, up to a level where the conditions are such that the wave dissipates and transfers energy to the background flow. This transfer of energy or momentum influences the speed and direction of the background flow and plays a role in the quasi-biennial oscillation (QBO) in the mean zonal wind in the tropical stratosphere below 35 km. Higher up in the atmosphere, the dissipation of the Kelvin waves contributes to the semi-annual oscillation (SAO) seen in the mean zonal wind in the upper stratosphere (above 35 km) and lower mesosphere.

The Kelvin waves induce fluctuations in zonal and vertical velocities, geopotential height and temperature. Furthermore, fluctuations in concentrations of trace gases are induced through the velocity perturbations and the temperature dependence of the photochemical reactions producing or destroying the respective trace gases. A more detailed description of the Kelvin wave theory and an overview of Kelvin wave observations are given in chapter 2.

1.3 Diabatic descent in the polar vortices

The solar radiation flux on the surface is higher at the equator of the Earth than it is at the poles. The atmosphere therefore is heated more at the equator and a temperature and pressure gradient is formed between the equator and the poles. The
warm high pressure air at the equator will move towards the poles as to decrease the pressure gradient and because of the rotation of the Earth (the Coriolis force) the air will bend off, relative to the ground, and will be moving also in the East direction. This bending off effect is larger at higher latitudes and so the zonal velocity of the air (from West to East) will be larger closer to the poles. This process causes a whirlpool-like meandering current around the globe called the polar-jet. In winter when the temperature gradient is larger, the polar jet becomes stronger. The polar-jet encloses a region of air centered at the poles called the polar vortex. When the polar jet is strong enough it prevents the mixing of air from inside and outside the polar vortices.

The mean meridional circulation, the Brewer-Dobson circulation, is driven by the dissipation of planetary and gravity waves and associated transfer of momentum and heat from the waves to the mean flow. The Brewer-Dobson circulation is characterised by upward motion in the tropics, a poleward flow in the winter hemisphere stratosphere and downward motion at high latitudes (see Figure 1.3). In the polar vortex descending flow compresses the air. This increase in pressure of air parcels adiabatically warms the air parcels above their radiative equilibrium temperature. To return to this radiative equilibrium temperature the air parcels increase the emission of long-wave radiation leading to a decrease in the potential temperature of the air parcels. This is called diabatic cooling or descent. Since concentrations of long-lived species are conserved in air parcels undergoing dynamical processes, diabatic descent and ascent rates can be inferred by tracking constant concentrations of long-lived species (see Figure 6.12).

Figure 1.3: Brewer Dobson circulation in Southern hemisphere winter.
1.4 Satellite measurements

Since the 1960’s a large number of Earth observational satellites have been launched. The main purpose of the earliest satellites was to study the weather from space. But also from the 60’s the first attempts to measure ozone were performed. In later years, the capabilities of the satellite instruments improved and the number of atmosphere parameters retrieved from satellite instruments kept growing. Over the last decade Earth observing satellites have proven their capabilities to accurately monitor nearly all aspects of the total Earth system on a global basis [CEOS, 2002].

The main advantages of satellite measurements are that (i) they provide a global overview, which is especially advantageous over the oceans and sparsely populated land areas, (ii) uniformity, since the same sensor measures at many different places, (iii) they are relatively uniformly distributed over the globe, (iv) performed on a regular time basis and (v) often span a number of years.

There are two types of satellite orbits: geostationary and polar orbiting (see Figure 1.4). Geostationary satellites in principle have a fixed position above a point at the
equator. The altitude of the geostationary satellites is around 40,000 km. They perform detailed observations of a specified region, and because of their fixed position have a good coverage in time. Polar orbiting satellites circle over the poles around the Earth, normally at an altitude lower than 2000 km and higher than 600 km. They offer the possibility to take measurements from the equator to high latitudes, in some cases up to the poles. Often these polar orbiting satellites cross the equator at the same local time every day. This is important when the instruments on the satellite require sunlight to perform a measurement. These orbits are named sun-synchronous orbits.

Satellite instruments mostly measure electromagnetic radiation. This can be done in a passive way, i.e. the instruments measure the solar or terrestrial radiation emitted, transmitted or reflected by an object, or in an active way, i.e. the sensor provides its own source of electromagnetic radiation and the interaction with the object is measured (e.g. radar). The electromagnetic radiation interacts with the atmosphere, therefore the measured radiation contains information on the state of the atmosphere. Different types of radiative processes play a role: extinction, scattering and absorption-emission. These are illustrated in Figure 1.5 (from Stephens [1994]).
Figure 1.5: Three types of interactions between electromagnetic radiation and the atmosphere (in this case a cloud): (a) extinction, (b) emission, (c) scattering.

Variables that are measured by means of satellite instruments are: the composition of the atmosphere (i.e. concentrations of trace gases), concentrations and characteristics of particles in the atmosphere (aerosols), temperature, pressure, density, cloud properties, ocean waves, snow cover, plate tectonics, biological activity, vegetation types and many others. In this thesis only one of these many types of satellite applications have been used: concentrations of trace gases in the atmosphere. In the next sections two satellite instruments, GOME and ILAS, will be described in more detail. Measurements by these two instruments have been used in the studies described in this thesis.

1.4.1 The GOME instrument

The GOME instrument was launched on board the second European Remote Sensing Satellite (ERS-2) on 21 April 1995. Its main objective is to measure the concentrations of atmospheric trace gases, which play an important role in the ozone chemistry [Burrows et al., 1999]. The ERS-2 has been put into a polar, sun-synchronous orbit at an altitude of 780 km, with a local crossing time at the equator of 10:30 AM for the descending node.

GOME scans the Earth across-track making a forward scan from east to west followed
by a backscan from west to east. The forward scan lasts 4.5 seconds and consists of three pixels with an area coverage of $40 \times 320 \text{ km}^2$ each, when using the maximum swath width of 960 km. The backscan lasts 1.5 seconds and covers an area of $40 \times 960 \text{ km}$. Global coverage is reached in three days when the instrument is operated with a maximum swath width.

The GOME instrument is a passive four-channel spectrometer that measures the radiation from the sun that is scattered by the Earth’s atmosphere or reflected from the surface of the Earth (Earth radiance). Additionally for calibration the radiation coming directly from the sun (solar irradiance) is measured. The spectral range is 240 to 790 nm with a resolution between 0.2 and 0.4 nm. From the ratio of the Earth Radiance and the solar irradiance, which is named the reflectivity, total column amounts of several trace gases are retrieved utilizing their characteristic spectral absorption. For example ozone has a very characteristic absorption pattern between 310 and 350 nm, called the Huggins band.

Figure 1.6 shows the total ozone column distribution from one day of measurements (21 September 2000). The orbit of the satellite can be seen as well as the ozone hole above the South Pole. In this thesis total column amounts of ozone are used but also vertical profiles of ozone. The steep rise of ozone absorption from 350 to 265 nm also offers the possibility to derive information on the vertical distribution of ozone [Twomey, 1961]. Shortwave radiation gets strongly absorbed by ozone and does not reach the lower layers of the atmosphere while radiation with a longer wavelength is not so strongly absorbed and can partly reach lower levels in the atmosphere. Radia-
tion at a short wavelength can thus be used to derive information on the upper layers of the atmosphere and radiation at longer wavelengths provides information on the lower layers of the atmosphere.

The emphasis of GOME is on ozone, but GOME also offers the possibility to derive abundances of other trace gases, such as nitrogen dioxide (NO₂), water vapour (H₂O), aerosols, formaldehyde (HCHO), sulphur dioxide (SO₂), bromine oxide (BrO) and the chlorine species OCIO [Valks, 2003; Richter and Burrows, 2002; Wagner and Platt, 1998; Eisinger and Burrows, 1998].

1.4.2 The ILAS instrument

The ILAS instrument was launched on board the Advanced Earth Observing Satellite (ADEOS) on August 17, 1996. It obtained 8 months of data from 1 November 1996 until 30 June 1997, when a solar panel failure caused the end of the ADEOS mission. The main goal of the ILAS instrument was to monitor and study the stratospheric ozone layer in both the high latitude regions in the Northern and Southern hemispheres.

ADEOS was placed in a sun-synchronous orbit and circled the Earth about fourteen times a day. During each of these orbits ILAS measured the sunlight reaching the sensor through the atmosphere by looking at the sun during sunrise over the Northern high-latitude region and during sunset over the Southern high-latitude region (see Figure 1.7). This observation method is called the solar occultation technique. The measurements during sunset and sunrise and the change in the position of the Earth relative to the sun within a year lead to a latitudinal coverage as shown in Figure 1.8. The amount of absorption of sunlight and the wavelengths at which the absorption takes place are different for each trace gas in the atmosphere. This makes it possible to derive the concentration of trace gases by measuring the absorption at different wavelengths. Because ILAS tracks the sun at sunset and sunrise as seen from the instrument, it measures the transmitted sunlight at different tangent heights which enables the retrieval of vertical distributions of atmospheric constituents. The retrieval is based on non-linear least squares fitting for spectral fitting and the onion peeling method for vertical profiling [Yokota et al., 1998].
1.5 This thesis

As mentioned in the introduction, this thesis examines two different dynamical processes that take place in the atmosphere, making use of satellite measurements. The greater part of the thesis, chapters 2 to 5, is focused on the detection of equatorial Kelvin waves by using satellite measurements of ozone concentrations. Although Kelvin waves play an important role in the dynamics of the middle atmosphere, the climatology of the waves is still not very well known. Ground-based observations do not provide a global picture of the waves and satellite measurements are generally limited by their vertical resolution or limited continuous operating periods. The GOME dataset used in this study covers more than 7 years. The goal of this work is to demonstrate the potential of the GOME data set to contribute to a global desc-
tion of Kelvin wave activity. The derived detected wave signatures can furthermore provide a tool to check the quality of the GOME ozone retrievals in the tropics.

A smaller part of the thesis is focused on the determination of diabatic descent and ascent rates in the polar vortices by using satellite measurements of nitrous oxide (N$_2$O). These diabatic descent and ascent rates are necessary for corrections in trajectory calculations, which are used for validation studies.

The following questions are addressed throughout this thesis:

- Can Kelvin waves be detected in total ozone column and ozone profile measurements from GOME?
- Is the vertical resolution of the vertical ozone profiles from GOME sufficient to provide information on the vertical structure of the Kelvin wave activity?
- How well do the Kelvin wave signals in the GOME measurements agree with Kelvin wave signals in temperature and wind data from the European Centre for Medium-Range Weather Forecasts (ECMWF)?
- Can the diabatic descent or ascent rates in the polar vortices be determined from ILAS measurements of N$_2$O?

The thesis starts with a more elaborate description of Kelvin waves in chapter 2: what are the forces controlling the waves, what are the governing equations, how are they formed and how do they propagate and break down, what are the characteristics, where can they be found and what previous observations have been documented?

The three following chapters consist of three papers, published in or submitted to the Journal of Geophysical Research. The first paper (chapter 3) is aimed at detecting Kelvin waves in total ozone columns from GOME. In the second paper (chapter 4) the results from the first paper are brought in relation with Kelvin wave analyses of temperature and zonal wind data from the ECMWF Re-analysis dataset. This dataset is produced by combining observations with a model. The third paper (chapter 5) then deals with the possibility of detecting Kelvin wave signals in GOME ozone profiles, and results will again be related to the Kelvin wave signals in the ECMWF data.

The second atmospheric process that is studied is described in chapter 6. This chapter deals with the determination of diabatic descent and ascent rates from ILAS measurements of N$_2$O. This work is part of two papers titled: “Use of potential vorticity coordinates and trajectories to increase the spatial coverage of satellite measurements: application to ILAS V5.20” and “Comparison of diabatic heating rates calculated using ILAS N2O data and a radiative transfer model”. First authors of these papers are respectively G. Bodeker and H. Struthers from the National Institute of Water and Atmospheric research (NIWA), situated in Lauder, New Zealand. The papers will shortly be submitted to Geophysical Research Letters.
Equatorial Kelvin waves

2.1 Introduction

Planetary scale equatorial waves play a significant role in the dynamics of the stratosphere and lower mesosphere. Forced by unsteady convective heating the waves propagate horizontally and vertically and herewith carry momentum into the upper atmosphere. The transfer of momentum from the waves to the background flow contributes to the driving of global circulations such as the quasi-biennial oscillation in the lower stratosphere and the semi-annual oscillation in the upper stratosphere and mesosphere. This chapter focuses on one specific type of equatorial wave: the equatorial Kelvin wave. It is an eastward propagating wave with a vanishing meridional velocity perturbation. The Kelvin wave induces perturbations in geopotential height, zonal and vertical velocity and temperature. Through these perturbations, the Kelvin wave also causes perturbations in concentrations of trace gases, e.g. ozone. This can happen both through transport effects and through the temperature dependence of photochemical reactions producing or destroying the trace gases.

This chapter starts in section 2.2 by explaining the linear wave theory applicable to Kelvin waves and showing the structure of the waves. Sections 2.3 and 2.4 discuss the forcing and absorption of Kelvin waves in the atmosphere. The last section, section 2.6 treats observed Kelvin waves and their characteristics.

2.2 Linear wave theory

The basic equations describing equatorial waves can be derived from the linearised momentum balance, continuity, hydrostatic balance and thermodynamic equations, neglecting non conservative processes [Andrews et al., 1987]. This leads to the following equations:

$$\frac{\partial u'}{\partial t} - \beta v' + \frac{\partial \psi'}{\partial x} = 0$$

(2.1)

This chapter has been prepared using the general reference books: Holton [1992], Andrews et al. [1987] and Holton et al. [2003]. Additional references are given in the text.
Equatorial Kelvin waves

\[
\frac{\partial u'}{\partial t} + \beta y u' + \frac{\partial \Phi'}{\partial y} = 0
\] (2.2)

\[
\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \rho_0^{-1} \frac{\partial (\rho w')}{\partial z} = 0
\] (2.3)

\[
\frac{\partial \Phi'}{\partial z} = H^{-1} RT' 
\] (2.4)

\[
\frac{\partial \Phi'}{\partial t} + \frac{\partial \Phi}{\partial z} w' = 0
\] (2.5)

The zonal wind \( u \), meridional wind \( v \), vertical velocity \( w \), geopotential height \( \Phi \), temperature \( T \) and potential temperature \( \Theta \) are all split up into a time and longitude-averaged mean, indicated with an overbar and a wave perturbation indicated with a prime, e.g. \( u = \bar{u} + u' \). \( \rho_0 \) is the standard density, \( R \) is the gas constant for dry air (= 287 \ JK^{-1} \ kg^{-1}), \( \kappa = R/c_p \), \( c_p \) is the specific heat at constant pressure and \( H \) is the scale height, which is \( \approx 7 \) km in the middle atmosphere. \( x, y, z \) are respectively the longitudinal, zonal and vertical coordinates. \( \bar{u} \) is set to zero.

Since we are looking at waves that are confined around the equator, the equatorial plane approximation can be used. In this approximation the Coriolis parameter \( f \) is replaced by \( y/(2a) \), \( a \) is the earth’s radius and \( y \) is the distance north of the equator.

Solutions to equations (2.1)-(2.5) can be written in the form:

\[
(u', v', w', \Phi') = e^{z/2H} R e \left[ (\bar{u}(y), \bar{v}(y), \bar{w}(y), \bar{\Phi}(y)) \exp i (kx + mz - \omega t) \right] 
\] (2.6)

Here \( k \) and \( m \) are the zonal and vertical wavenumbers respectively and \( \omega \) is the angular frequency.

The simplest solution for \( (\bar{u}(y), \bar{v}(y), \bar{w}(y), \bar{\Phi}(y)) \) is found when taking \( \bar{v} = 0 \). This solution where the meridional velocity perturbation vanishes is the equatorial Kelvin wave.

Substituting equation (2.6) into equations (2.1)-(2.4) then gives us:

\[
-\omega \bar{u} + k \Phi = 0 
\] (2.7)

\[
\beta y \bar{u} + \Phi_y = 0 
\] (2.8)

\[
k \bar{u} - \omega N^{-2} (m^2 + \frac{1}{4H^2}) \Phi = 0 
\] (2.9)

where \( \rho_0 = \rho_s e^{z/H} \), \( \rho_s \) being the density at the surface. \( N \) is the buoyancy frequency, which is defined as:

\[
N^2 = \frac{R}{H} \left[ \frac{\partial T}{\partial z} + \frac{\kappa T}{H} \right] = \frac{R}{H} \beta z e^{-\kappa z/H} 
\] (2.10)

Equations (2.7) and (2.9) give us \( \omega = \pm Nkm^{-1} \). For the vertical group velocity we then get: \( c_g^z \equiv \partial \omega / \partial m = \mp Nkm^{-2} \). Positive group velocity corresponds to
waves propagating upward and therefore will be the physical solution, thus giving the dispersion relationship:

\[ \omega = -Nk/m \]  \hspace{1cm} (2.11)

The meridional structure of the Kelvin wave solution can be found by combining equations (2.7) and (2.8):

\[ \Phi(y) = \Phi_0 \exp \left( -\beta y^2 / 2 \omega \right) = \Phi_0 \exp \left( -\beta y^2 / 2c \right) \]  \hspace{1cm} (2.12)

where \( \Phi_0 \) is the amplitude of the wave in geopotential height at the equator and \( z=0 \) and \( c \) is the phase speed \( \equiv \omega / k \).

If the amplitude of the wave has to decay going away from the equator, the coefficient in the exponent in (2.12) has to be negative and thus the phase velocity \( c \) has to be positive. Therefore, Kelvin waves are eastward propagating. Furthermore from (2.11) we conclude that \( m \) must be negative. Phase surfaces \( (kx + mz - \omega t) \) tilt eastward with height and move downward with time as can be seen in Figure 2.1.

\[ C_g, \text{direction of energy propagation} \]

\[ t=t_1 \]

\[ t=t_2 \]

\[ \theta = \text{constant} \]

\[ \text{Wavefront propagation} \]

\[ \text{Material line} \]

\[ \text{Height} \]

\[ \text{Longitude} \]

\[ \text{W} \]

\[ \text{E} \]

\textbf{Figure 2.1}: Direction of phase speed \( c \) and group velocity \( c_g \).

Using (2.12) the wave solutions are given by:

\[ u' = \frac{k}{\omega} \Phi_0 \exp \left( -\beta y^2 / 2 \omega \right)e^{z/2H} Re \left[ \exp \ i(kx + mz - \omega t) \right] \]  \hspace{1cm} (2.13)

\[ \Phi' = \Phi_0 \exp \left( -\beta y^2 / 2 \omega \right)e^{z/2H} Re \left[ \exp \ i(kx + mz - \omega t) \right] \]  \hspace{1cm} (2.14)

\[ T' = \frac{H}{R} \Phi_0 \exp \left( -\beta y^2 / 2 \omega \right)e^{z/2H} Re \left[ \left( \frac{1}{2H} + im \right) \exp \ i(kx + mz - \omega t) \right] \]  \hspace{1cm} (2.15)
The latter one is derived from the hydrostatic equation (2.4). The zonal velocity, geopotential and temperature perturbations vary in latitude as Gaussian functions centered on the equator. The e-folding decay width is given by

\[ Y_K = \sqrt{2c/\beta} \]  

(2.16)

which is about 15° at the equator for a phase speed of 30 m/s typical for lower stratospheric Kelvin waves.

\[ u f + \frac{dp}{dy} \]

\[ u' f' + \frac{dp'}{dy} \]

**Figure 2.2:** Plan view of the geopotential height and zonal velocity perturbations for the equatorial Kelvin wave. H and L denote locations of maximum and minimum geopotential height perturbations.

The structure of the geopotential height and zonal velocity perturbations for the Kelvin wave are shown in plan view in Figure 2.2. The meridional force balance controlling the equatorial Kelvin wave is an exact balance between the meridional pressure gradient and the zonal velocity (see Figure 2.3). Because of the change of sign of the Coriolis parameter at the equator, this force balance and thus the equatorial Kelvin wave can exist. The structure of the wave in the xz plane is the same as for an internal gravity wave. Figure 2.4 shows a longitude-height section of the velocity,
pressure and temperature perturbations along the equator. For a Kelvin wave with $|m| \gg \frac{1}{H}$, temperature perturbations will lead the zonal wind perturbations by 1/4 of a cycle. This so-called "Boussinesq" approximation is reasonable for 'slow' Kelvin waves in the lower stratosphere.

Equations (2.1)-(2.4) are valid for $\bar{u} = 0$. For a nonzero but constant $\bar{u}$, these equations are somewhat more extensive but the solutions (2.13) - (2.15) can be easily adapted by replacing $\omega$ with the intrinsic frequency $\omega^+ = \omega - ku$.

### 2.3 Forcing

Equatorial Kelvin waves are thought to be forced by the latent heat release, which is associated with organised cumulus convection. Observed Kelvin waves in the lower stratosphere are mainly of zonal wavenumber 1 with wave periods of about 10 to 20 days. However, the heat sources thought to force the Kelvin waves do not show a large spectral peak at these frequencies [Wallace and Chang, 1972]. Apparently the atmosphere acts like a band-pass filter that primarily lets through specific frequencies, even if the heat sources forcing the waves are distributed randomly in the frequency domain.

Holton [1973] demonstrated that the specific observed Kelvin wave frequencies may
follow from the natural wave response of the atmosphere in conditions favorable for Kelvin wave modes i.e. in the presence of downward propagating westerlies, independently of the spectral character of the forcing. Furthermore, Chang [1976] showed that the vertical scale of convective heating determines a selective frequency response, favoring modes whose vertical wavelengths are twice that of the forcing. It was also demonstrated that for randomly distributed tropospheric heat sources, the lowest zonal wavenumbers are excited most efficiently.

2.4 Absorption

Different mechanisms can lead to the dissipation of equatorial Kelvin waves. One of them is when the waves reach a so-called critical level. The eastward propagating waves can penetrate through westward flow. Near levels where the westward flow shifts to an eastward flow, the upward group velocity and vertical wavelength decrease as the intrinsic speed (\(= c - \bar{u} \)) and intrinsic frequency go to zero. The approach to the critical level is slowed so that wave transient is extended indefinitely causing strong interaction between the waves and the mean flow. The decreasing group velocity furthermore leads to effective dissipation of the waves.

Another mechanism is damping by e.g. radiative cooling or small scale turbulence. Again when the upward group velocity of the Kelvin wave decreases rapidly, dissipative processes can break up the wave. Both mechanisms result in a transfer of energy and momentum from the waves to the background flow. This gives the Kelvin wave an important role in the circulation of the atmosphere.

2.5 Importance of equatorial Kelvin waves

The equatorial Kelvin wave influences the atmosphere in several ways [Holton et al., 2003]. The waves are an important source of large-scale temperature variability in the tropical stratosphere and mesosphere. They can rapidly carry information eastward, thereby creating easterly trade winds. This is an effective way to homogenise the atmosphere in zonal direction. The large scale cooling associated with Kelvin waves can generate and maintain tropical tropopause cirrus. Furthermore stratospheric ozone can be transported to the troposphere by either downward motion associated with the Kelvin waves or by wave breaking around the tropopause.

But, the most important influence of Kelvin waves is seen when the waves dissipate and transfer momentum to the background flow. This source of momentum influences the strength and direction of the mean circulation and with this play a role in the forcing of two major wind oscillations in the atmosphere: The Quasi-Biennial Oscillation (QBO) and the Semi-Annual Oscillation (SAO). The first one is a cycle in the lower and middle stratosphere equatorial winds with a period of about 27 months. The winds show alternating descending eastward and westward wind regimes. Figure 2.5 shows the driving of the QBO by vertically propagating waves. In Figure 2.5a the mean zonal wind is westward. While westward waves (e.g. Rossby-Gravity waves) cannot penetrate the westward shear zone, eastward waves (e.g. Kelvin waves) can propagate to higher altitudes before getting absorbed. The dissipation of the waves at higher altitudes causes an eastward acceleration of the mean flow. In Figure 2.5b it
is illustrated that after a certain time a weak eastward flow appears aloft the layer of westward flow in the lower layers. The eastward waves can penetrate the lower layers and deposit eastward momentum at and above the transition level between westward and eastward flow. This will bring down the lower base level of the eastward flow and increase the strength of the eastward flow above this level. In Figure 2.5c the limit is reached where the lower layer of westward flow cannot descend any further and the layer with eastward flow is located immediately above the the lower westward jet. At this point the lower jet decays and eventually vanishes, probably through vertical diffusion of momentum. Then the westward waves are free to propagate vertically and create a new westward acceleration at upper levels, as is shown in Figure 2.5d. The whole process repeats itself in the other direction until the situation in Figure 2.5a recurs. This makes up an entire cycle of the QBO. The SAO is a similar oscillation in the equatorial zonal winds above 35 km in the upper stratosphere and lower
mesosphere. It has a period of about 6 months. Kelvin waves together with westward moving Rossby-Gravity waves and gravity waves can force the SAO in a similar way as for the QBO by depositing momentum and causing accelerations in the mean zonal flow.

2.6 Observations of equatorial Kelvin waves

2.6.1 Kelvin wave induced fluctuations

Kelvin waves modulate geopotential height, velocity, both zonal and vertical, and temperature. In addition Kelvin waves also induce fluctuations in the concentrations of ozone and other trace gases. So Kelvin waves can be observed in measurements of velocity and temperature but also measurements of trace constituents can be used to identify Kelvin waves. Short-lived species which are temperature sensitive will respond to Kelvin wave temperature fluctuations through chemical adjustment. Long-lived species on the other hand will respond to Kelvin wave motions through dynamical adjustment. Especially the constituents having strong vertical gradients will be affected by the vertical motions of the Kelvin wave.

For ozone this means that in the upper stratosphere where ozone has a short chemical lifetime and a temperature dependent equilibrium concentration, fluctuations are primarily caused by the temperature dependence of the photochemical reactions producing and destroying ozone. In this region the ozone and temperature perturbations are out of phase. Contrary, in the lower atmosphere ozone has a strong vertical gradient and a long photochemical lifetime, thus fluctuations in this region are primarily transport related. In this case, the ozone and temperature perturbations are in phase [Salby et al., 1990]. Largest ozone fluctuations are found where the amplitude of the temperature perturbations and the vertical gradient in ozone is large.

2.6.2 Characteristics

In the observations three main types of Kelvin waves are distinguished according to their phase speed. As the Kelvin waves propagate vertically, thermal dissipation preferentially absorbs slow components, letting faster components through. Therefore higher up in the atmosphere more rapidly propagating Kelvin waves dominate.

Table 2.1 shows the 3 types of Kelvin waves and gives some characteristics for each type for zonal wavenumber 1.

Furthermore there also seems to be evidence of ultraslow Kelvin waves with periods of 25-30 days in the lowest part of the tropical stratosphere [Canziani, 1999]. Observations in which more than one frequency range has been observed simultaneously indicate that there appear to be discrete preferred frequency ranges with a clear separation between them [Smith et al., 2002]. Note that because Kelvin waves are non dispersive zonally, the Kelvin waves have frequencies in wave number 2 which are approximately twice those of their counterparts in wave number 1.
2.6 Observations of equatorial Kelvin waves

<table>
<thead>
<tr>
<th></th>
<th>Slow Kelvin Wave</th>
<th>Fast Kelvin Wave</th>
<th>Ultra Fast Kelvin wave</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase speed (m/s)</td>
<td>20-40</td>
<td>60</td>
<td>120</td>
</tr>
<tr>
<td>Period (days)</td>
<td>10-20</td>
<td>6-10</td>
<td>3-4</td>
</tr>
<tr>
<td>Region</td>
<td>LS</td>
<td>MS, US</td>
<td>US, M, LT</td>
</tr>
<tr>
<td>Latitudinal width (°)</td>
<td>30</td>
<td>40</td>
<td>50</td>
</tr>
<tr>
<td>Vertical wavelength (km)</td>
<td>10</td>
<td>20</td>
<td>40</td>
</tr>
</tbody>
</table>

Table 2.1: Different types of Kelvin waves and their characteristics for zonal wavenumber 1. LS= lower stratosphere; MS= middle stratosphere; US= upper stratosphere; M= mesosphere; LT= lower thermosphere.

2.6.3 Observational studies

One of the earliest observational studies on Kelvin waves was done by Wallace and Kousky [1968]. Using wind and temperature measurements from radiosondes they identified "slow" Kelvin waves in the lower stratosphere with periods of about 2 weeks. Hirota [1978] made use of rocketsonde temperature and wind observations to show evidence of the "fast" Kelvin waves in the upper stratosphere and mesosphere with periods of about 7 days. Since these studies Kelvin waves have been subject of many studies using ground based measurements such as radiosondes or ozonesondes [e.g. Holton et al., 2001; Boehm and Verlinde, 2000; Fujiwara et al., 2003, 2001, 1998]. Unfortunately there are very few stations near the equator that provide wind, temperature and or trace gas measurements on a regular basis.

With the availability of satellite observations, the global structure of the Kelvin waves has been investigated. Fast Kelvin waves were identified in the temperature and ozone measurements from the Limb Infrared Monitor of the Stratosphere (LIMS) and Solar Backscatter Ultraviolet (SBUV) instruments on board the Nimbus-7 spacecraft [Salby et al., 1984, 1990; Randel, 1990; Randel and Gille, 1991] and the Improved Stratospheric And Mesospheric Sounder (ISAMS) [Stone et al., 1995] and Microwave Limb Sounder (MLS) [Canziani et al., 1994, 1995; Mote and Dunkerton, 2002] on board the Upper Atmosphere Research Satellite (UARS).

Slow Kelvin waves in the lower stratosphere need observations with a sufficiently high vertical resolution to get resolved. They have been observed in temperature and ozone profiles retrieved from measurements by LIMS [Kawamoto et al., 1997], MLS [Mote and Dunkerton, 2004] and Cryogenic Limb Array Etalon Spectrometer (CLAES) [Shiotani et al., 1997; Canziani, 1999; Mote and Dunkerton, 2004], the latter two on board UARS. The limited (continuous) time periods covered by the LIMS, MLS and CLAES measurements do however not allow the study of the variability of slow Kelvin waves over more than two years and by that the conjunction with the QBO cycle. This statement is also valid for the study by Smith et al. [2002], who identified both high and low frequency wave signals in temperature and trace gas measurements from the Cryogenic Infrared Spectrometers and Telescopes for the Atmosphere (CRISTA) instrument. This instrument operates on a free-flying satellite launched and retrieved by the Space Shuttle. Data was analysed from two flights, each lasting a week.

Ziemke and Stanford [1994] found tropical Kelvin wave signatures in the Nimbus-7 TOMS (Total Ozone Mapping Spectrometer) total column ozone data, and herewith
Equatorial Kelvin waves showed that total ozone column measurements also appear to be sensitive to slow Kelvin waves in the lower stratosphere.
Equatorial Kelvin wave signatures in ozone column measurements from GOME

abstract
This study investigates tropical Kelvin wave signatures in the total ozone column data from the Global Ozone Monitoring Experiment (GOME) instrument. A new approach for spectral analysis is introduced by generalizing an unequally spaced data technique from one to two dimensions. This enables the handling of satellite data containing gaps. The simple statistical behavior of the method furthermore allows an easy determination of the statistical significance of any observed spectral features. Seven years of GOME data (1995-2002) have been analyzed in which we have identified three periods of high Kelvin wave activity in 1996, 1998 and 2000. The periods are in conjunction with westward equatorial zonal winds at 30 hPa and show eastward propagating waves 1-2 with periods of ~ 12-15 days. The induced Kelvin wave signatures in the ozone concentrations are around 2-4 DU peak-to-peak, and can be attributed to 'slow' Kelvin waves. The results are shown to be significant.

Our study provides an important contribution to the study of Kelvin waves by introducing the bi-dimensional unequally spaced data spectral analysis and is the first to demonstrate the potential of the GOME ozone data set to contribute to a global description of equatorial Kelvin wave activity.

3.1 Introduction

Planetary scale equatorial waves play an important role in the dynamics of the tropical atmosphere. Forced by large-scale unsteady convective heating and accompanying latent heat release, these waves propagate horizontally and vertically carrying momentum into the middle and upper atmosphere.

The Kelvin wave is one of the most dominant equatorial waves. The change in sign of the Coriolis parameter at the equator allows this special type of equatorial wave to exist. It is an eastward propagating wave characterized by zonal velocity and geopotential perturbations varying in latitude as Gaussian functions centered at the equator. The waves also induce temperature fluctuations because of adiabatic heating and cooling when air parcels are vertically displaced. The observed Kelvin waves are primarily of zonal wave number 1 or 2 and have periods in the lower stratosphere of about 15 days [Holton, 1992]. Furthermore, Kelvin waves are mainly detected when the mean flow is westward because waves are absorbed or reflected when their phase velocity is in the same direction as the background current and only waves that head against the current can penetrate it. Thus, in case of a mean westward flow, the eastward heading Kelvin waves can propagate into the middle and upper stratosphere. There they are absorbed, and the eastward momentum carried upward by the Kelvin waves is transferred to the background flow. The transfer of momentum causes an eastward acceleration of the current and eventually a reverse from westward to eastward. The reversal in the winds begins in upper levels and propagates downward in time. The same process takes place for the westward traveling Rossby-gravity waves but in the opposite direction. The Rossby-gravity waves penetrate the eastward mean zonal flow carrying westward momentum upward into the upper stratosphere where the momentum is transferred to the background current. The momentum provided by the Kelvin and Rossby-gravity waves together with gravity waves is believed to be responsible for driving the quasi-biennial oscillation (QBO) of the zonal mean winds in the lower stratosphere and the semi-annual oscillation (SAO) in the upper stratosphere and mesosphere [Canziani and Holton, 1998, and references herein]. Both these oscillations are important features in the global circulation.

In addition to temperature fluctuations, Kelvin waves also induce fluctuations in the ozone concentrations. In the upper stratosphere where ozone has a short chemical lifetime and a temperature dependent equilibrium concentration, this takes place through the temperature dependence of the photochemical reactions. In the lower atmosphere where ozone has a strong vertical gradient and a long photochemical lifetime this takes place through motions. Thus both temperature as well as ozone observations can be used to identify Kelvin waves.

One of the earliest observational studies on Kelvin waves was done by Wallace and Kousky [1968]. Using wind and temperature measurements from radiosondes they identified "slow" Kelvin waves in the lower stratosphere with periods of about 2 weeks. Hirota [1978] made use of rocketsonde temperature and wind observations to show evidence of the "fast" Kelvin waves in the upper stratosphere and mesosphere with periods of about 7 days.

With the availability of satellite observations, the global structure of the Kelvin waves has been investigated. Fast Kelvin waves were identified in the temperature and ozone measurements from the Limb Infrared Monitor of the Stratosphere (LIMS) and Solar Backscatter Ultraviolet (SBUV) instruments on board the Nimbus-7 spacecraft [Salby et al., 1984, 1990; Randel, 1990; Randel and Gille, 1991] and the Improved Stratospheric And Mesospheric Sounder (ISAMS) [Stone et al., 1995] and Microwave Limb Sounder (MLS) [Canziani et al., 1994, 1995] on board the Upper Atmosphere Research Satel-
Slow Kelvin waves in the lower stratosphere need observations with a sufficiently high vertical resolution to get resolved. They have been observed in temperature and ozone profiles retrieved from measurements by LIMS [Kawamoto et al., 1997] and Cryogenic Limb Array Etalon Spectrometer (CLAES) [Shiotani et al., 1997; Canziani and Holton, 1998], the latter on board UARS. The limited time periods covered by the LIMS and CLAES measurements do however not allow the study of the variability of slow Kelvin waves over more than two years and by that the conjunction with the QBO cycle.

Total ozone column measurements also appear to be sensitive to slow Kelvin waves in the lower stratosphere. Ziemke and Stanford [1994] found tropical Kelvin wave signatures in the Nimbus-7 TOMS (Total Ozone Mapping Spectrometer) total column ozone data covering November 1978 to January 1992. Observed periods for zonal waves 1-2 were ~5-15 days with amplitudes of the induced ozone perturbations around 3 DU. This is in agreement with model calculations presented in the same study suggesting that Kelvin waves should dynamically induce total ozone perturbations of a few DU.

Reproducing a realistic QBO and Kelvin waves in atmospheric models has been proven to be difficult [Pawson, 1992; Takahashi, 1996, 1999; Hamilton et al., 1999]. However, many improvements are being made. Amodei et al. [2001] compared tropical oscillations and planetary scale Kelvin waves in four troposphere-stratosphere climate models and the assimilated data set produced by the United Kingdom Meteorological Office (UKMO). None of the four models reproduced a wind structure that resembles the QBO. Despite this, all four models are able to generate Kelvin waves with amplitudes close to those observed in the MLS and CLAES data in the lower stratosphere. In three of the models the absence of a QBO allows Kelvin waves to propagate up into the upper stratosphere and mesosphere, where their amplitude grows. Consequently, the Kelvin wave amplitudes in these three models are overestimated in the upper stratosphere and mesosphere.

This present study shows that the GOME ozone column data exhibit features that can be attributed to tropical Kelvin waves. Three periods have been identified with high Kelvin wave activity. The significance of the results has been verified by statistical analysis.

In spite of their importance in the atmosphere, a climatology of tropical Kelvin waves does not exist. This study demonstrates the potential of the GOME measurements to contribute to the derivation of such a climatology.

3.2 GOME measurements

The Global Ozone Monitoring Experiment (GOME) instrument flies on board of the second European Remote Sensing Satellite (ERS-2), which was launched on April 21st 1995. GOME is a nadir viewing spectrometer that measures the direct solar irradiance and the solar radiation scattered by the Earth’s atmosphere and surface in the ultraviolet and visible wavelength range of 240 to 790 nm at a spectral resolution of 0.2-0.4 nm. GOME scans the Earth surface with a spatial resolution of 40 km in latitudinal and 320 km in longitudinal direction. Global coverage is reached within
3 days. Total ozone column values are retrieved from the ratio of the radiance and irradiance spectra by utilizing the characteristic spectral absorption of ozone in part of the Huggins band (325-335 nm). The technique used for the retrieval is based on the DOAS (Differential Optical Absorption Spectroscopy) method [Platt, 1994; Burrows et al., 1999]. The amount of ozone below the cloud top, which is called the ghost vertical column, can not be detected by GOME and is therefore derived from a climatological ozone profile.

For this study we have used GOME GDP (GOME Data Processing) version 2.7 total ozone column data [Spurr et al., 2002].

The accuracy of the retrieved ozone columns in the tropics is of particular importance for this study. The relative error (precision) of the GDP 2.7 total ozone is of the order of 1% (Shown by data assimilation, Eskes et al. [2003]). Comparison of GOME total ozone columns with Brewer and Dobson measurements shows differences smaller than 3% in the tropics [Balis et al., 2001]. The agreement between the GOME and TOMS total ozone measurements is generally good [Bramstedt et al., 2002; Lambert et al., 2000]. However, at the equatorial latitudes TOMS values are ~3-5% higher than both GOME and TOVS (TIROS Operational Vertical Sounder) ozone columns [Corlett and Monks, 2001]. The multi spectral DOAS method used in the GOME ozone retrieval has several advantages compared to the TOMS algorithm which is based on wavelength pairs and triplets [McPeters et al., 1998; Martin et al., 2002; Valks et al., 2003]. The GOME algorithm is less sensitive to aerosols and deviations from the assumed surface albedo.

3.3 Analysis method

The ozone column measurements from GOME are taken at variable latitudes and longitudes. To obtain an ozone time series on a fixed latitude-longitude grid we have defined a set of 5° × 5° grid cells covering the latitude band from 2.5° S to 2.5° N and all longitudes. This latitude band is chosen because the Kelvin waves reach maximum amplitude at the equator. For each grid cell we collect all cloud-free measurements in a 3 day period with center coordinates within the grid cell and compute the average ozone density.

We have only used the cloud-free ground pixels (cloud fraction < 0.1), since GOME measurements in case of clouds suffer from uncertainties in the ghost vertical column, as described above. About half of the total number of GOME measurements in the tropics are cloud-free, resulting in about 5-40 measurements per grid cell over a period of 3 days. Averaging over these measurements increases the precision of the used values from ~1% to ~0.2-0.5%. A possible bias in the data will be filtered out by the spectral analysis and will thereby not influence the results.

In the past several different spectral techniques have been applied to detect Kelvin wave signals in satellite measurements, most of them based on the Fourier transform, which is applied to switch from a representation of the data as function of time and space to a representation of the data as function of wave number and frequency. To determine which wavenumbers and frequencies are dominant in the data, the periodogram can be calculated, which is defined as the spectral power (square of the Fourier amplitude) as function of angular frequency ω and zonal wave number k.
3.3 Analysis method

In this study we have used a method of spectral analysis developed by Lomb [Press et al., 1992], and further elaborated by Scargle [1982]. This method of spectral analysis can be applied to unevenly sampled data, and was first used in Canziani [1999]. Satellite data sets often contain gaps both in space and time which are not easily handled. The use of interpolation techniques to fill in the gaps are generally not satisfactory. For example, long gaps in the data can produce misleading power at low frequencies corresponding to wavelengths comparable to the gaps [Press et al., 1992]. The method developed by Lomb (which we will call Lomb periodogram) can be applied to unevenly sampled data without the use of interpolation techniques, it simply evaluates the data at the actually measured locations and times. Another important reason to use this technique is its favorable statistical behavior, explicated below, which permits the evaluation of the reliability of an observed spectral signal.

Consider a variable \( h \) measured at times \( t_j \) with \( j=1,2,...,N \). The classical periodogram in one dimension, based on discrete Fourier transformation (DFT), is then defined as:

\[
P(\omega) \equiv \frac{1}{N} \left[ \sum_{j=1}^{N} h(t_j) \cos \omega t_j \right]^2 + \left[ \sum_{j=1}^{N} h(t_j) \sin \omega t_j \right]^2
\]  

(3.1)

In case of even sampling (time between consecutive measurements is constant), the statistical distribution of this periodogram is simple and makes it easy to determine the significance of an observed spectral feature. In contrary, when the data are sampled at arbitrary \( t_j \)'s, the statistical distribution is much more complicated. The Lomb periodogram is a modified version of the classical periodogram that does have a simple statistical behavior even in the case of uneven sampling. Again consider the variable \( h \) measured at times \( t_j \) with \( j=1,2,...,N \). The Lomb normalized periodogram in one dimension is then defined as:

\[
P_N(\omega) \equiv \frac{1}{2\sigma^2} \left[ \frac{\left[ \sum_{j} (h_j - \bar{h}) \cos(\omega(t_j - \tau)) \right]^2}{\sum_j \cos^2(\omega(t_j - \tau))} + \left[ \sum_{j} (h_j - \bar{h}) \sin(\omega(t_j - \tau)) \right]^2}{\sum_j \sin^2(\omega(t_j - \tau))} \right]
\]  

(3.2)

with

\[
\tau = \frac{1}{2\omega} \text{atan} \left[ \frac{\sum_j \sin(2\omega t_j)}{\sum_j \cos(2\omega t_j)} \right] \quad \text{(3.3)}
\]

\[
\bar{h} = \frac{1}{N} \sum_{j=1}^{N} h(t_j) \quad \text{(3.4)}
\]

\[
\sigma^2 \equiv \frac{1}{N-1} \sum_{j=1}^{N} (h(t_j) - \bar{h})^2 \quad \text{(3.5)}
\]

Because we are dealing with GOME data in two dimensions, i.e. as function of time and longitude, we have extended the Lomb method from one to two dimensions. We consider a two dimensional data set consisting of \( N_{\text{tot}} \) data points. The functional
value is denoted by \( h_{j,l} \equiv h(t_j, x_l) \) measured at times \( t_j \) with \( j = 1, 2, ..., N_t \) and locations \( x_l \) with \( l = 1, 2, ..., N_x \). The Lomb normalized periodogram as function of angular frequency \( \omega \) and zonal wave number \( k \) is given by:

\[
P_N(\omega, k) \equiv \frac{1}{2\sigma^2} \left[ \frac{\sum_{j,l}(h_{j,l} - \bar{h})\cos(\omega(t_j - \tau_1) \pm k(x_l - \tau_2))}{\sum_{j,l}\cos^2(\omega(t_j - \tau_1) \pm k(x_l - \tau_2))} \right]^2 
+ \frac{\sum_{j,l}(h_{j,l} - \bar{h})\sin(\omega(t_j - \tau_1) \pm k(x_l - \tau_2))}{\sum_{j,l}\sin^2(\omega(t_j - \tau_1) \pm k(x_l - \tau_2))} \right]^2
\]

(3.6)

with

\[
\tau_1 = \frac{1}{2\omega} \arctan \left[ \frac{\sum_l \sin 2\omega t_l}{\sum_l \cos 2\omega t_l} \right]
\]

(3.7)

\[
\tau_2 = \frac{1}{2k} \arctan \left[ \frac{\sum_l \sin 2k x_l}{\sum_l \cos 2k x_l} \right]
\]

(3.8)

\[
\bar{h} \equiv \frac{1}{N_{tot}} \sum_{j=1}^{N_t} \sum_{l=1}^{N_x} h(x_l, t_j)
\]

(3.9)

\[
\sigma^2 \equiv \frac{1}{N_{tot} - 1} \sum_{j=1}^{N_t} \sum_{l=1}^{N_x} (h(x_l, t_j) - \bar{h})^2
\]

(3.10)

The plus sign in equation (3.6) corresponds to westward traveling waves and the minus sign to eastward traveling waves.

Because the periodogram of noisy data also is noisy, it can exhibit large spurious peaks that should not be mistaken for a periodic signal. Therefore it is necessary to evaluate the significance of an observed spectral peak in the periodogram. The statistical significance of a spectral peak is found by considering the probability that it could have arisen from noise fluctuations. We have chosen for the Lomb normalized periodogram because this probability is easily determined from the simple statistical behaviour of the Lomb periodogram even in the case of unequally spaced data. In case \( h_{j,l} \) would be pure Gaussian noise, \( P_N \) at any particular \( \omega \) and \( k \) is exponentially distributed with unit mean. Hence, the probability that \( P_N(\omega, k) \) for arbitrary \( \omega \) and \( k \) will lie between \( z \) and \( z + dz \) is \( \exp(-z)dz \). If we scan \( M \) independent frequencies, the probability that none give values larger than \( z \) is \( (1 - e^{-z})^M \). So the probability that one frequency gives a peak larger than \( z \) is:

\[
Pr(> z) \equiv 1 - (1 - e^{-z})^M
\]

(3.11)

A small value of this probability means there is a small chance that the peak is caused by noise and thus indicates a highly significant periodic signal. Equation (3.11) leads to the following detection threshold \([\text{Scargle}, 1982]\):

\[
z_0 = -\ln \left[ 1 - (1 - p_0)^{\frac{1}{M}} \right]
\]

(3.12)
3.4 Results

An observed power exceeding this detection threshold $z_0$ has a $p_0$ probability of being caused by pure noise. Accordingly, using $p_0 = 0.01$, a power exceeding $z_0$ indicates a 99% significant periodic signal.

3.4 Results

Figure 3.1 shows the periodogram $P_N$ as function of wave number and period for three 60-day time periods (P1: 15 July-13 September 1996; P2: 17 July-15 September 1998; P3: 19 September-18 November 2000).

To detect a specific wave period, a sufficiently long time series is needed which covers several times this wave period [Priestley, 1989]. However, choosing a time period length that is much longer than the period in which the Kelvin waves are active will reduce the signal from the Kelvin waves. Taking into account these two counteracting factors, experimenting with different lengths of the time periods used in our calculations learned that 60 days is a suitable length for this study. The blue, green and red areas respectively denote the 90%, 99% and 99.9% significant signals. All three time periods show significant signals corresponding to eastward propagating waves 1-2 with periods of 15 days (1996, 1998) and 12 days (2000). These signatures agree with Kelvin wave characteristics.

For comparison Figure 3.2a shows the periodogram $P_N$ for time period P3 using total ozone columns from EP-TOMS averaged over 3 days on a $5° \times 5°$ mesh. The results are comparable to the results from the GOME GDP in Figure 3.1, only with a maximum at slightly longer wave periods of about 12-15 days.

To check our significance criteria we have also calculated the periodogram using random data, see Figure 3.2b. As anticipated the periodogram does not exceed the 90% significance level at any wave number and period. When repeating the experiment numerous times, the periodogram hardly ever exceeds the 90% significance level and in none of the repetitions exceeds the 99% significance level (the probability for this is 1%).

To compare our method with a more standard spectral approach we have also applied the Lomb periodogram to the Nimbus-7 TOMS total ozone column data analysed in Ziemke and Stanford [1994]. For this, the TOMS ozone columns are averaged over 1 day and regridded to a $5° \times 5°$ mesh. Figure 3.2c shows the results for the period from 15 July to 13 September 1984. The plot shows a dominating signal from eastward waves 1 and 2 with periods between 8 and 30 days, which is in good agreement with the spectral amplitudes calculated by Ziemke and Stanford for the same period (see figure 2a, period E2 in their paper).

To find all episodes of high Kelvin wave activity in the 7-year time period from the start of the GOME operation in July 1995 until July 2002, we have plotted in Figure 3.3 the periodogram $P_N$, calculated over 60-day time periods, for wave 1 at two specific frequencies corresponding to wave periods of 12 and 15 days, as function of the starting date of the 60-day periods. The solid horizontal lines indicate the 90%, 99% and 99.9% significance levels. This figure clearly shows episodes of highest wave activity with wave periods of 15 days in 1996 and 1998, corresponding to the previously defined P1 and P2 periods, and an episode of highest wave activity with wave periods of 12 days in 2000, corresponding to period P3.
NCEP reanalysis data [Kalnay et al., 1996] of monthly mean zonal winds at 30 hPa for the same 7-year time period have been used to identify periods where strong Kelvin wave activity is expected. Figure 3.4 shows the zonal wind at 30 hPa at the equator. Periods P1, P2 and P3 are indicated with arrows. A clear correlation can be seen, especially in 1996 and 1998, between the wave activity and the westward zonal wind. This is in agreement with previous studies [Shiotani and Horinouchi, 1993], in which it was found that westward zonal wind at 30 hPa shows an in-phase

Figure 3.1: Lomb periodogram for the GOME ozone columns for 3 different periods.

Figure 3.2: Lomb periodogram for a) the 3-day averaged TOMS ozone columns in period P3 b) random data and c) the 1-day averaged TOMS ozone columns in the period from 15 July to 13 September 1984.
Figure 3.3: Time series of Lomb Periodogram for wave 1 at two specified frequencies. Upper plot corresponds to a wave period of 12 days and lower plot to a wave period of 15 days. The periodogram is plotted as function of the starting day of the 60-day time periods over which the periodogram is calculated.
relationship with lower stratospheric Kelvin wave activity.

Figure 3.4 shows time versus longitude plots (commonly known as Hovmöller diagrams) for the three episodes P1, P2 and P3. The data are filtered as to retain only waves 1 and 2. Furthermore, in time a band-pass filter given by Murakami [1979] is applied with half amplitudes at 10 and 15 days. This filtering is applied to separate out the dominant frequencies shown in Figure 3.1. The Hovmöller diagrams give information on the propagation of waves with the selected frequencies, amplitudes of the ozone variations induced by these waves and can be used to determine the phase velocity of the waves. The plots reveal movements of the highest amplitudes that are eastward. The amplitudes are in the order of 1-2 DU, in agreement with model calculations by Ziemke and Stanford [1994]. The phase velocity of the waves, determined by taking the slope of lines through the amplitude maxima or minima, is between 25-45 m/s.

Observed ozone perturbations are in the same order of magnitude as the noise in the 3-day averaged and gridded ozone columns (section 3.3). However this noise is distributed over all spatial and temporal frequencies in contrast to the Kelvin wave signatures which correspond to particular scales, i.e. specific frequencies and wave numbers [Salby et al., 1990]. Only the fraction of the noise operating on those specific scales is relevant. If the error variance is distributed over all frequencies then the signal is an order of magnitude above the noise. Would this not be the case then it would be difficult to explain the signatures found at the specific frequencies and wave numbers corresponding to the dispersion characteristics of the equatorial Kelvin waves.
3.5 Outlook

The spectral analysis method introduced in this paper can be applied to other satellite measurements.

The total ozone record of GOME is extended by SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) [Bovensmann et al., 1999], which is an extended version of GOME, launched on board ENVISAT in March 2002 and from 2005-2020 by the GOME-2 series on the METOP 1, 2 and 3 platforms.

Combining the GOME total ozone record with the data from the SCIAMACHY and GOME-2 missions are anticipated to provide a 25-year time series of ozone column data (1995-2020) that allows the construction of a climatology of stratospheric Kelvin wave activity. A combination with the TOMS Nimbus-7 and Meteor-3 ozone column data sets (1978-1994) could be used to extend this time series. This however requires an homogenization of the two data sets.

The features found in the GOME total ozone columns can be attributed to ‘slow’ Kelvin waves in the lower stratosphere. However, profile measurements are needed to detect the vertical distribution of the Kelvin waves. Profile measurements also allow the same analysis, shown in this paper for total ozone columns, on separate stratospheric layers. Ozone profiles retrieved from the GOME nadir measurements [Van der A. et al., 2002] will be analyzed to determine whether they can be used to detect Kelvin wave perturbations.

In addition to nadir measurements, the SCIAMACHY instrument also performs limb measurements that will provide ozone profile data with a vertical resolution of ~3 km. The instrument observes the same airmass in limb and nadir viewing geometries within about 7 minutes. A combination of nadir column and limb profile measurements will offer the possibility for a better description of the 3-dimensional distribution of equatorial Kelvin wave activity.

Figure 3.5: Hovmöller diagrams of waves 1&2 for time periods P1, P2 and P3. A band-pass filter with half-amplitudes at 10 and 15 days has been applied. Solid lines start at zero DU with an increment of 0.5 for each contourline. Dashed lines start at -0.5 DU with a decrement of 0.5 for each contourline.
3.6 Conclusion

The extension of the unequally spaced data spectral technique first developed by Lomb from one to two dimension makes it possible to analyse two dimensional datasets while profiting from the advantages of the Lomb periodogram. The main advantages are the applicability to unequally spaced data, like satellite data with gaps in space and time, and the possibility to evaluate the significance of observed spectral features.

By applying this new method to seven years of GOME total ozone column measurements, we found spectral features which can be attributed to equatorial Kelvin waves in the lower stratosphere. These features are shown to be significant by exploiting the statistical behavior of the method.

Three periods of high Kelvin wave activity have been identified in 1996, 1998 and 2000, which correlate to periods of westward equatorial zonal winds at 30 hPa. The three periods show eastward propagating waves 1-2 with periods of 12-15 days and induced ozone column variations around 2-4 DU peak-to-peak. The results agree with the characteristics of ‘slow’ Kelvin waves in the lower stratosphere. The method has also been applied to TOMS ozone column data and shows results comparable to the results from using GOME data.

This study makes a new contribution in the field of Kelvin wave analysis by introducing bi-dimensional unequally spaced data spectral analysis and demonstrates the sensitivity of the GOME ozone columns to tropical Kelvin waves, showing the potential of the GOME ozone measurements to contribute to a global description of equatorial Kelvin wave activity.

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4

Kelvin wave signatures in ECMWF meteo fields and GOME ozone columns

abstract
This study investigates the vertical structure of the Kelvin wave signals previously found in total ozone column measurements from the GOME instrument. For this, zonal wind and temperature measurements from the European Centre for Medium-Range Weather Forecasts (ECMWF) Re-Analysis dataset are analysed by using the same bi-dimensional spectral method as was used to analyse the GOME total ozone columns. These fields are available on 60 levels from the surface to 0.1 hPa. For the three high Kelvin wave activity periods identified in the GOME data we found spectral features in the ECMWF fields associated with Kelvin waves with zonal wavenumbers 1 or 2 and periods around 15-20 days. These characteristics correspond to the characteristics of the Kelvin waves detected in GOME. The signals are significant throughout the lower stratosphere between ~ 100-10 hPa and depending on the period are largest around 15, 45 or 65 hPa. There is a good correlation between the Kelvin wave signals in the ECMWF zonal wind and temperature and the GOME total ozone column. The induced fluctuations in zonal wind and temperature are respectively up to 8 m/s and 2 K. From these induced zonal wind fluctuations expected total ozone column fluctuations of around 1 DU are calculated, corresponding to the ozone fluctuations found in the GOME data. The results indicate that the analysed total ozone column fluctuations are mainly caused by transport effects in the lower stratosphere. This study shows that combined use of ECMWF Re-Analysis data and GOME ozone columns provides a possibility to study the 3-dimensional structure of Kelvin wave activity.

4.1 Introduction
Equatorial Kelvin waves play a significant role in the dynamics of the middle atmosphere. The main forcing mechanism of these waves is likely the latent heat release

in large-scale deep convection [Holton, 1992]. The waves propagate vertically and zonally in eastward direction through the atmosphere, and in this way can carry momentum into the middle and upper atmosphere. This process is believed to play a large role in the driving of the quasi-biennial oscillation (QBO) of the zonal mean winds in the lower stratosphere and the semi-annual oscillation (SAO) in the upper stratosphere and mesosphere. Kelvin waves are also thought to play a role in the stratospheric dehydration mechanism [Fujiwara et al., 2001; Fujiwara and Takahashi, 2001] and the transport of stratospheric ozone into the troposphere [Fujiwara et al., 1998].

A Kelvin wave modulates geopotential height, zonal velocity and vertical velocity and also temperature through the diabatic heating and cooling of the vertical displacements. The Kelvin wave also induces fluctuations in the ozone concentration. In the lower stratosphere, where ozone has a strong vertical gradient and a long photochemical lifetime, the ozone perturbations are mainly controlled through the velocity modulations. Conversely, in the upper stratosphere ozone has a short chemical lifetime and a temperature dependent equilibrium concentration. The ozone fluctuations in this part of the atmosphere are therefore mainly controlled by the temperature dependence of the photochemical reactions.

Wallace and Kousky [1968] were one of the first to observe Kelvin waves in the atmosphere. They used wind and temperature measurements from radiosondes and identified Kelvin waves in the lower stratosphere with periods of about 2 weeks, referred to as ‘slow Kelvin waves’. Later on several studies have analysed Kelvin waves in wind, temperature and ozone profile measurements by both ground-based and satellite instruments. In these studies, distinction is made between ‘ultra-slow’, ‘slow’, ‘fast’, and ‘ultra-fast’ Kelvin waves with phase speeds of respectively $\sim 10$-20 m/s, $\sim 25$-30 m/s, $\sim 70$ m/s and $\sim 120$ m/s. Satellite observations allow the investigation of the global structure of Kelvin waves. Fast Kelvin waves were identified in the temperature and ozone measurements from the Limb Infrared Monitor of the Stratosphere (LIMS) and Solar Backscatter Ultraviolet (SBUV) instruments on board the Nimbus-7 spacecraft [Salby et al., 1984, 1990; Randel, 1990; Randel and Gillett, 1991] and the Improved Stratospheric And Mesospheric Sounder (ISAMS) [Stone et al., 1995] and Microwave Limb Sounder (MLS) [Canziani et al., 1994, 1995; Mote and Dunkerton, 2002] on board the Upper Atmosphere Research Satellite (UARS). Slow Kelvin waves in the lower stratosphere need observations with a sufficiently high vertical resolution to get resolved. They have been observed in temperature and ozone profiles retrieved from measurements by LIMS [Kawamoto et al., 1997], MLS [Mote and Dunkerton, 2004] and Cryogenic Limb Array Etalon Spectrometer (CLAES) [Shiotani et al., 1997; Canziani, 1999; Mote and Dunkerton, 2004], the latter two on board UARS. The limited (continuous) time periods covered by the LIMS, MLS and CLAES measurements do however not allow the study of the variability of slow Kelvin waves over more than two years and by that the conjunction with the QBO cycle.

The studies (e.g. Kawamoto et al. [1997] and Mote and Dunkerton [2004]) that treat ozone Kelvin waves show dominant ozone mixing ratio variations at the level where the vertical gradient in zonal mean ozone is largest. These variations are attributed to dynamical advection of ozone and are in phase with temperature variations. A second maximum in ozone variability due to Kelvin waves is often found in the upper
4.2 Data and analysis

stratosphere, attributable to photochemical perturbations. These variations show an out of phase relationship with temperature variations.

Ziemke and Stanford [1994] showed that also total column measurements of ozone are sensitive to 'slow Kelvin waves' in the stratosphere. They found Kelvin wave signatures in the Nimbus-7 TOMS (Total Ozone Mapping Spectrometer) data.

In a previous study Timmermans et al. [2004] (hereinafter T04) demonstrated that GOME (Global Ozone Monitoring Experiment) ozone column measurements too exhibit features that can be attributed to tropical Kelvin waves. By introducing bi-dimensional unequally spaced data spectral analysis we analysed seven years of GOME data and identified three periods of high Kelvin wave activity. The induced Kelvin wave signatures in the ozone concentrations of 2-4 DU peak-to-peak correspond to eastward propagating waves 1-2 with periods of 12-15 days. These results agree with the characteristics of 'slow' Kelvin waves in the lower stratosphere. However no additional vertical information on the Kelvin waves can be retrieved from the total column ozone measurements themselves.

To acquire more information on the vertical structure of the Kelvin waves we will in this study correlate the variations in the GOME total column ozone data to variations in the European Centre for Medium-Range Weather Forecasts (ECMWF) Re-Analysis (ERA-40) zonal wind and temperature data, available at different altitudes. We will first analyse the ERA-40 data in the three high Kelvin wave activity periods identified in the ozone column data. Using these analyses we will compute the expected total ozone column perturbations and compare these with the ozone column perturbations found in T04.

4.2 Data and analysis

4.2.1 GOME

The Global Ozone Monitoring Experiment (GOME) instrument is a nadir-viewing spectrometer on board the second European Remote Sensing Satellite (ERS-2), which was launched on 21 April 1995. From the measured radiance and irradiance spectra, total ozone column values are retrieved with a global coverage in 3 days. The spatial resolution is 40 km in latitudinal and 320 km in longitudinal direction. For a more extensive description of the GOME data and its accuracy we refer to T04 and references herein.

4.2.2 The ECMWF Re-Analysis dataset, ERA-40

The ECMWF ERA-40 dataset consists of a set of global fields describing the state of the atmosphere (the "analysis"). These fields are produced by combining atmospheric observations with a forecast model using data assimilation [Simmons and Gibson, 2000]. The dataset covers the period from September 1957 to August 2002. The observations come from a wide selection of sources: radiosondes, aircraft, ground-based and satellite instruments; each of these measurements with their own accuracy. To obtain a complete representation at all locations and times, the measurements are combined with results from a short-range forecast initiated from the preceding analysis. The observations and forecast are then combined using estimates of the
statistics of their errors to form the new analysis. Every 6 hours a new analysis is made.

For this study we use the temperature and zonal and meridional wind fields from the ERA-40 dataset. We retrieved these three fields from the ECMWF dataset on a $5^\circ \times 5^\circ$ grid (resolution of original data T159) and average over 3 days (if not stated otherwise) to match the used GOME ozone fields. From this grid we have subsequently focused on the latitude band between $2.5^\circ$ S and $2.5^\circ$ N because Kelvin waves reach maximum amplitude at the equator. All results presented below are for this latitude band. The fields are available on 60 levels between the surface and 0.1 hPa. The vertical resolution is highest in the planetary boundary layer and lowest in the stratosphere and lower mesosphere. The model levels are calculated in relation to the surface pressure. An example of the pressure on the 60 levels for a surface pressure of 1015 hPa is given in Table 1. Between 40 and 4 hPa the level spacing is precisely 1.5 km. In the lower stratosphere, the level spacing is between 1 and 1.5 km. This vertical resolution should be sufficient for the detection of slow Kelvin waves, considering typical vertical wavelengths of these waves of about 8-10 km.

Tindall [2003, 2004b] investigated the representation of equatorial waves in ERA-15 data. In this study it is demonstrated that the Kelvin wave activity in the ERA-15 data show seasonal and interannual variations consistent with previous studies using other datasources. For example maximum Kelvin wave activity at 50 hPa coincides with the change in the zonal wind at this altitude from easterlies to westerlies. This is consistent with the results from Shiotani et al. [1997] and references herein. Other

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Table 4.1: ERA-40 pressure levels for a surface pressure of 1015 hPa.
studies have found equatorial waves in ERA-15 to be representative of the atmosphere. Straub and Kiladis [2002] for example found Kelvin wave signals in ERA-15 in agreement with signals in radiosonde data. Furthermore Pawson and Fiorino [1998] found a good agreement in the annual temperature cycle at 100 and 70 hPa between data from ERA-15 and radiosondes. All these studies give an indication of the reliability of ERA-15 data in terms of Kelvin waves. Although in this study we are using ERA-40 data instead of ERA-15, the conclusions from these studies are expected to be similar for the ERA-40 data. The main changes in ERA-40 compared to ERA-15 are the length of the dataset (40 years instead of 15) and the improved vertical resolution. This improved vertical resolution should be advantageous for the detection of Kelvin waves.

4.2.3 Analysis method

In this study we have used the bi-dimensional spectral analysis method introduced in T04. This method can handle unequally spaced data, such as satellite data containing gaps, without making use of interpolation techniques, which can introduce spurious peaks in the power spectrum. The simple statistical behavior of the method, allowing easy determination of the statistical significance of an observed feature, is another important advantage of the method.

The spectral method is based on the Lomb periodogram [Press et al., 1992; Scargle, 1982]. In T04 this periodogram is extended from one to two dimensions as to allow its application to the bi-dimensional GOME data (as function of longitude and time). The periodogram gives an indication of the dominant frequencies in a dataset. For each level in the ERA-40 data separately, we calculate the extended Lomb normalized periodogram as function of angular frequency \( \omega \) and zonal wave number \( k \).

4.3 Linear Kelvin wave theory

In this section we will derive the solutions for Kelvin wave induced perturbations in zonal wind, geopotential height and temperature using linear wave theory. Following Andrews et al. [1987] the basic equations for describing equatorial waves are given by:

\[
\frac{\partial u'}{\partial t} - \beta v' + \frac{\partial \Phi'}{\partial x} = 0 \quad (4.1)
\]

\[
\frac{\partial v'}{\partial t} + \beta u' + \frac{\partial \Phi'}{\partial y} = 0 \quad (4.2)
\]

\[
\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \rho_0^{-1} \frac{\partial (\rho_0 u')}{\partial z} = 0 \quad (4.3)
\]

\[
\frac{\partial \Phi'}{\partial z} = H^{-1} RT' \quad (4.4)
\]

The primes denote wave perturbations in zonal wind \( u \), meridional wind \( v \), vertical velocity \( w \), geopotential height \( \Phi \) and temperature \( T \). \( \rho_0 \) is the standard density, \( R \) is the gas constant for dry air \( (= 287 J K^{-1} kg^{-1}) \) and \( H \) is the scale height, which is
38 Kelvin waves in ERA-40 and GOME

≈ 7 km in the middle atmosphere. x, y, z are respectively the longitudinal, zonal and vertical coordinates.

These equations are derived from the linearised momentum balance, continuity and hydrostatic balance equations, neglecting non conservative processes. All field variables are split up into a time and longitude-averaged mean, indicated with an overbar and a wave perturbation e.g. u = \tilde{u} + u'. \tilde{u} is set to zero. Since we are dealing with latitudinally confined waves, the equatorial -plane approximation has been used in which the Coriolis parameter f is replaced by \beta y (\beta = 2\Omega^2a^{-1}, a is the earth’s radius and y is the distance north of the equator).

Solutions to equations (4.1)-(4.4) can be written in the form:

\[(u', v', w', \Phi') = e^{z/2H}Re \left( (\tilde{u}(y), \tilde{v}(y), \tilde{w}(y), \Phi(y)) \exp i(kx + mz - \omega t) \right) \]  

Here k and m are the zonal and vertical wavenumbers respectively and \omega is the angular frequency. Different solutions can be found for (\tilde{u}(y), \tilde{v}(y), \tilde{w}(y), \Phi(y)) which satisfy equations (4.1)-(4.4). The simplest one where we take \tilde{v} = 0 concerns the Kelvin wave. In this case \tilde{u} and \Phi have to satisfy the following relationships:

\[-\omega \tilde{u} + k \Phi = 0 \tag{4.6} \]
\[\beta y \tilde{u} + \Phi_y = 0 \tag{4.7} \]
\[k \tilde{u} - \omega N^{-2}(m^2 + \frac{1}{4H^2})\Phi = 0 \tag{4.8} \]

These relationships are derived by substituting equation (4.5) into equations (4.1)-(4.4) and using \rho_0 = \rho_s e^{z/H}, where \rho_s is the density at the surface. The buoyancy frequency N is defined as:

\[N^2 = \frac{\beta}{H} \left[ \frac{\partial T}{\partial z} + \frac{\kappa T}{H} \right] \tag{4.9} \]

with \kappa = \frac{R}{c_p}, and c_p is the specific heat at constant pressure.

The meridional structure of this wave solution can be found by combining equations (4.6) and (4.7):

\[\Phi(y) = \Phi_0 \exp (-\beta ky^2/2\omega) \tag{4.10} \]

where \Phi_0 is the amplitude of the wave in geopotential height at the equator and z=0. The wave solutions are then given by [Tindall, 2003; Tindall et al., 2004a]:

\[u' = \frac{k}{\omega} \Phi_0 \exp (-\beta ky^2/2\omega)e^{z/2H}Re \left[ \exp i(kx + mz - \omega t) \right] \tag{4.11} \]
\[\Phi' = \Phi_0 \exp (-\beta ky^2/2\omega)e^{z/2H}Re \left[ \exp i(kx + mz - \omega t) \right] \tag{4.12} \]
\[T' = \frac{H}{R} \Phi_0 \exp (-\beta ky^2/2\omega)e^{z/2H}Re \left[ \left( \frac{1}{2H} + im \right) \exp i(kx + mz - \omega t) \right] \tag{4.13} \]

The latter one is derived from the hydrostatic equation (4.4). For a Kelvin wave with | m | \gg \frac{1}{2H}, temperature perturbations will lead the zonal wind perturbations by 1/4 of a cycle. This so-called "Boussinesq" approximation is reasonable for 'slow' Kelvin waves in the lower stratosphere.
From equations (4.6) and (4.8) we get \( \omega = \pm Nkm^{-1} \) and the vertical group velocity \( c_g^{(z)} \equiv \partial \omega / \partial m = \mp Nkm^{-2} \). For an upward propagating Kelvin wave the positive \( c_g^{(z)} \) will be the physical solution and the dispersion relationship is given by:

\[
\omega = -Nk/m
\]

Equations (4.1) - (4.4) are valid for \( \bar{u} = 0 \). For a nonzero but constant \( \bar{u} \), these equations are somewhat more extensive but the solutions (4.11) - (4.14) can be easily adapted by replacing \( \omega \) with the intrinsic frequency \( \omega^{+} = \omega - ku \).

### 4.4 Results

In the previous study T04 we found in the GOME ozone column data three periods of high Kelvin wave activity: P1 from 15 July to 13 September 1996, P2 from 17 July 1998 to 15 September 1998 and P3 from 19 September 2000 to 18 November 2000. These three periods correlate with periods of westward zonal winds in the lower stratosphere as can be seen in Figure 4.1.

Below we show the results of the analyses of the ERA-40 zonal wind and temperature data concentrating on these three periods.

**P1: 15 July to 13 September 1996**

Figure 4.2 shows the periodogram \( P_{N} \) as function of wavenumber and period for the ECMWF temperature, zonal and meridional wind velocity at 15 hPa calculated over the 60-day time period from 15 July to 13 September 1996. This time period corresponds to the time period P1 in T04.

In both the temperature and zonal wind field one large significant eastward signal is found. This significant signal is located at wavenumbers 1 and 2 with periods around 15-20 days. This maximum corresponds to the signal found in the GOME total ozone data in T04 and agrees with Kelvin wave characteristics. The meridional wind field does not show a significant signal at these wavenumbers and periods, another indication that the signal is Kelvin wave related, since Kelvin waves do not have a meridional component. The signal is also present in the periodograms of the temperature and zonal wind at other altitudes between approximately 100 and 7 hPa, as can be seen in Figure 4.3. The signal in zonal wind is largest at \( \sim 20 \) hPa and in temperature at 35hPa for wave periods of 20 days and 15 hPa for wave periods of 15 days.

Figure 4.4 shows Hovmöller diagrams (time versus longitude plots) for the temperature, zonal and meridional wind fields at 15 hPa from 15 July to 13 September 1996. To produce this figure we used the daily values instead of the three day averaged values. The data are filtered as to preserve only the dominant frequencies found in the temperature and zonal wind periodograms that are expected to arise from Kelvin waves. The filter only retains wavenumbers 1 and 2. In time a band-pass filter given by Murakami [1979] is applied with half amplitudes at 12 and 20 days. From these figures we can retrieve the amplitudes of the wave perturbations in the wind velocity and temperature. At this level observed perturbations in the zonal wind are up to 8 m/s, in the temperature \( \sim 2 \) K. The perturbations in the meridional wind are negligible as expected from Kelvin wave theory. These values agree with the observed
Figure 4.1: Monthly mean zonal wind [m/s] at the equator and 105° E for January 1996 to December 2000 and pressure levels between 100 and 10 hPa. (Image provided by the NOAA-CIRES Climate Diagnostics Center, Boulder, Colorado, USA, from their Web site at http://www.cdc.noaa.gov/.)

Figure 4.2: Lomb periodogram for ERA-40 temperature, zonal and meridional wind, at 15 hPa for the period 15 July to 13 September 1996. Contourlines start at 2.5, followed by contourlines at 5, 10, 15, 20 and 25. The blue, green and red areas respectively denote the 90%, 99% and 99.9% significant signals.
4.4 Results

Figure 4.3: Lomb periodogram for ERA-40 temperature and zonal wind, for eastward waves with zonal wavenumber 1 for the period 15 July to 13 September 1996.

Figure 4.4: Hovmöller diagram of waves 1 and 2 in temperature, zonal and meridional wind velocity at 15 hPa. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at zero K (for temperature) or m/s (for zonal and meridional wind) with increments of 1 for each contour line. Dashed lines start at -1 K or m/s with a decrement of 1 for each contour line.

Values given in Andrews et al. [1987]. The wave period and phase speed determined from these Hovmöller diagrams are respectively 15 days and 31 m/s, which agrees with the characteristics of the slow Kelvin wave in the lower stratosphere.

Taking a cross section of these plots at a fixed time, as shown in Figure 4.5 for 10 September 1996, provides an image of the phase difference in space between the zonal wind and temperature perturbations. It can be seen that the zonal wind lags the temperature perturbations by a 1/4 cycle, which corresponds to the linear Kelvin wave theory explained in section 4.3. $\partial T/\partial x$ is thus in phase with the zonal wind perturbations as can be seen in this figure.

Figures 4.6 and 4.7 show pressure versus longitude and pressure versus time plots for the temperature and zonal wind perturbations, respectively on 23 August 1996 and at longitude=310°, the date and longitude where we found our maximum zonal
wind perturbation. A distinct wave 1 structure can be seen from approximately 200 to 5 hPa with an eastward phase tilt with height, characteristic for eastward moving Kelvin waves. Observed perturbations in these figures are up to 7 m/s for the zonal wind and 2K for the temperature, with largest values found between 10 and 20 hPa. Note that the largest amplitudes here are smaller than seen in the Hovmöller diagrams (Figure 4.4), this is caused by the three day averaging of the data here compared to the daily values used for producing the Hovmöller diagrams. Perturbations can also be seen below 200 hPa and above 5 hPa. These perturbations however do not show an eastward phase tilt with height and therefore can not be attributed to Kelvin waves.

Figure 4.8, a cross-section of the pressure versus longitude plots, shows the vertical structure of the zonal wind and temperature perturbations. The data are not filtered in the vertical direction, nevertheless a clear vertical wave structure can be seen in both the temperature and zonal wind plot, between approximately 100 hPa and 1 hPa, but note that above results showed that perturbations above 5 hPa can not be attributed to Kelvin waves. The lower boundary is set by the tropopause region where the Kelvin waves originate and the upper boundary by the level where the waves dissipate. In the figure we can again see the 1/4 cycle phase difference between the temperature and zonal wind perturbations, this time in the vertical. The vertical wavelength derived from these plots is $\sim 10$ km. The amplitude of the fluctuations increases up to 10 hPa and decreases above 10 hPa. In the linear Kelvin wave theory
Figure 4.6: Pressure versus longitude plots of waves 1 and 2 in temperature, zonal wind velocity on 23 August 1996. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 K (for temperature) and 0 m/s (for zonal wind) with increments of 0.5 K and 2 m/s for each contour line. Dashed lines start at -0.5 K or -2 m/s with a decrement of 0.5 K and 2 m/s for each contour line.

Figure 4.7: Pressure versus time (daynumber of the 60-day period 15 July to 13 September 1996) plots of waves 1 and 2 in temperature, zonal wind velocity at longitude=310°. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Values of contour lines are the same as in Figure 4.6.
Andrews et al. [1987] showed that Kelvin waves can only exist when their intrinsic phase velocity ($c - u_z$) is larger than 0 and thus when the phase velocity is larger than the mean background zonal wind $u_z$. In the presence of a vertical wind shear, the Kelvin waves will be able to propagate as long as $c > u_z$ up to a critical level where $c = u_z$. When approaching this critical level, the vertical wavelength and vertical group velocity will decrease and the waves become more susceptible to dissipation. This is what can be seen in Figure 4.8 around 10 hPa. The right plot in Figure 4.8 shows the mean zonal wind. The mean zonal wind becomes eastward between ~2.5 and 10 hPa and forms a critical level where dissipation of the waves take place. Above this level the Kelvin wave induced zonal wind and temperature perturbation are reduced. The signal in the periodograms of the temperature and zonal wind at wavenumbers 1-2 and periods of 15-20 days was also diminishing at altitudes above ~10 hPa, pointing to dissipation of the waves at this altitude. Also the decrease of vertical wavelength towards the critical level is visible in Figure 4.8. Large amplification of the amplitudes is observed in the region where westward winds change to eastward in agreement with previous studies (e.g. Shiotani et al. [1997] and Tindall et al. [2004b]).

Figure 4.9 shows for 1996 the normalised ozone column periodogram and the normalised zonal wind and temperature periodograms, for wave 1 with a waveperiod of 15 days. The thick dashed lines are the periodogram values for the zonal wind.
and temperature on the 15 hPa level, which is the level where we found the largest temperature and zonal wind perturbations. The correlation coefficient between the

![Figure 4.9: Normalised ozone column periodogram values P_N (solid line) and normalised zonal wind (upper plot) and temperature (lower plot) periodogram values, calculated over 60-day time periods, for wave 1 with a waveperiod of 15 days, as function of the starting day of the 60-day periods in 1996. The zonal wind and temperature periodograms are calculated on 11 different levels (dotted lines) between 80 hPa and 8 hPa. The thick dashed lines are the periodogram values on the 15 hPa level.](image)

ozone column periodogram and the zonal wind periodogram at 15 hPa is 0.63. The location of the peak in the ozone column periodogram coincides very well with the peak in the 15 hPa zonal wind and temperature periodograms. The 15 hPa zonal wind line follows the ozone line very well up till the peak mid July 1996. After this peak the periodogram for the zonal wind is higher than for ozone, thus in the zonal wind at 15 hPa there is more wave signal than in the ozone column. At some of the other altitudes however there is a lower wave signal after the peak than at 15 hPa. The correlation coefficient between the ozone column periodogram and the temperature periodogram at 15 hPa is 0.76. The 15 hPa temperature periodogram follows the ozone periodogram quiet well from February until the peak in mid July. After the peak we see the same situation as in the zonal wind plot. Also in January the 15 hPa temperature periodogram lies above the ozone column line, but again some other altitudes show periodogram values closer to the ozone column ones. An explanation for this could be that a wave signal in the ozone column requires a wave signal in most levels between 80 and 10 hPa. Similar correlation plots have been analysed for wave 1 with wave periods of 10, 12, 20 and 30 days. A good correlation was found
between the zonal wind, temperature and ozone column periodograms of waves with periods of 12 and 20 days. For the wave periods of 10 and 30 days the correlation was not very good.

All the analyses shown here for P1 (15 July to 13 September 1996) have also been performed for the two other periods (17 July 1998 to 15 September 1998 and 19 September 2000 to 18 November 2000) in which we found high Kelvin wave activity in the GOME ozone column data.

**P2: 17 July 1998 to 15 September 1998**
The results for P2 are somewhat similar to the results shown for the 1996 period. For P2 we found the maximum signal in the zonal wind and temperature periodograms of wave 1 with periods of 12-20 days at approximately 65 and 55 hPa (see Figure 4.10). The zonal wind and temperature periodograms at this level show a maximum around waves 1 and 2 with periods of 15 days, which is not present in the meridional wind.

Figures 4.11 and 4.12 are the same as Figures 4.6 and 4.7 but now for respectively 10 August 1998 and longitude=205°, the date and longitude where we find the largest Kelvin wave induced zonal wind perturbation (Note: larger perturbations are found between 1.0 and 0.1 hPa, however these perturbations do not show the characteristic eastward phase tilt with height and therefore can not be attributed to Kelvin waves).

The Kelvin wave induced zonal wind and temperature perturbations between ~100 and 3hPa are up to 3.8 m/s and 1.5 K respectively. Largest perturbations are again found around 10-20 hPa, furthermore large amplitudes can be found between 50-100 hPa, the altitude range where we found largest periodogram values. The vertical wavelength is about 10-12 km.

**P3: 19 September 2000 to 18 November 2000**
The results are similar to the results shown for the P1 and P2 period. The maximum signal in the zonal wind and temperature periodograms of wave 1 with periods of 12-20 days are found around 15-20 hPa (see Figure 4.13). The periodogram also shows a significantly large signal at altitudes above 10 hPa. As can be seen in Figure 4.1 the
4.4 Results

Figure 4.11: Pressure versus longitude plots of waves 1 and 2 in temperature, zonal wind velocity on 10 August 1998. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 K (for temperature) and 0 m/s (for zonal wind) with increments of 0.5 K and 2 m/s for each contour line. Dashed lines start at -0.5 K or -2 m/s with a decrement of 0.5 K and 2 m/s for each contour line.

Figure 4.12: Pressure versus time (daynumber of the 60-day period 17 July to 15 September 1998) plots of waves 1 and 2 in temperature, zonal wind velocity at longitude=205°. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Values of contour lines are the same as in Figure 4.11.
mean zonal winds in P3 are strongest around 15-20 hPa compared to maximum winds around 30 hPa for periods P1 and P2. Therefore period P3 may be more favorable for wave propagation higher up in the stratosphere. The zonal wind and temperature periodograms at 15-20 hPa show a maximum around waves 1 and 2 with periods of 15 days, which is not present in the meridional wind.

Figures 4.14 and 4.15 are the same as Figures 4.6 and 4.7 but now for respectively 1 October 2000 and longitude=180°. The Kelvin wave induced zonal wind and temperature perturbations are up to 5 m/s and 2 K respectively. Largest perturbations

Figure 4.13: Lomb periodogram for ERA-40 temperature and zonal wind, for zonal wavenumber 1 for the period 19 September to 18 November 2000. Contourlines start at 12.5 with an increment of 12.5 for each contourline.

Figure 4.14: Pressure versus longitude plots of waves 1 and 2 in temperature, zonal wind velocity on 1 October 2000. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 K (for temperature) and 0 m/s (for zonal wind) with increments of 0.5 K and 2 m/s for each contour line. Dashed lines start at -0.5 K or -2 m/s with a decrement of 0.5 K and 2 m/s for each contour line.
are found between 5 to 10 hPa, furthermore large amplitudes can be found between 10 to 20 hPa, the altitude where we found maximum periodogram values. The vertical wavelength is about 10-12 km.

4.5 Ozone column variations derived from ERA-40 u and T

The Kelvin wave variability in the ERA-40 zonal wind and temperature show very good agreement with the Kelvin wave variability previously found in the GOME total ozone column data. Next we will examine whether the fluctuations found in the ERA-40 data theoretically can lead to the fluctuations found in the total ozone columns. First we determine the fluctuations in the ozone mixing ratio resulting from the temperature and zonal wind fluctuations. For this we use the linearised tracer continuity equation [from Andrews et al., 1987, equation 9.4.4.]:

\[
\frac{\partial \chi'}{\partial t} + \bar{u} \frac{\partial \chi'}{\partial x} + w \frac{\partial \chi}{\partial z} = S_P
\]

(4.15)

where \( \chi \) is the tracer mixing ratio, primes denote wave perturbations and the overbar denotes the zonal mean. The net photochemical production/destruction \( S_P \) will be neglected in the following calculation. The analysed Kelvin wave fluctuations in the GOME ozone columns, show characteristics of the slow Kelvin waves in the lower stratosphere. In the lower stratosphere photochemical influences on ozone can be neglected by comparison with transport effects [Salby et al., 1990].
To solve $\chi'$ we also use the linearised thermodynamic equation as previously applied by Randel [1990], Salby et al. [1990] and Kawamoto et al. [1997]:

$$\left( \frac{\partial}{\partial t} + \bar{u} \frac{\partial}{\partial x} \right) T' + w' S = 0$$

(4.16)

where

$$S = \frac{1}{H} \left( \frac{2}{7} \bar{T} + \frac{\partial \bar{T}}{\partial z} \right)$$

(4.17)

is a background static stability parameter and the other variables as defined in section 4.2.3. Combining equations (4.16) and (4.15) leads to the following relation between the ozone and temperature fluctuations [Equation 9 in Salby et al., 1990]:

$$\chi' = \frac{\partial \chi}{S} T'$$

(4.18)

This equation states that when only considering transport effects, the induced ozone fluctuations are proportional to the vertical gradient in mean ozone and in phase with the temperature fluctuations for a positive vertical gradient of ozone. Note that in contrary in the upper stratosphere where photochemical effects dominate over transport effects the ozone fluctuations are out of phase [Salby et al., 1990].

In Figure 4.16 examples of the vertical distribution of ozone fluctuations calculated from equation (4.18) are shown. In the calculation the temperature fluctuations found in the ERA-40 data (filtered for zonal wavenumbers 1 and 2 and in time with time filter with half-amplitudes at 12 and 20 days) are used. $\partial \chi / \partial z$ has been derived from the AFGL (Air Force Geophysical Laboratory) standard atmosphere for the tropics (see Figure 4.17). The largest fluctuations in ppmv are located around 30 hPa where the vertical gradient in ozone is largest. Fluctuations in the mixing ratio of ozone above 10 hPa as can be seen in Figure 4.16c diminish when making the conversion to DU (see Figure 4.16e) and thus will not make a large contribution to the total ozone column fluctuations.

Using hydrostatic equilibrium the perturbations in the total column ozone $X_{tot}'$ in DU are given by

$$X_{tot}' = \frac{1}{2.69 \times 10^{16}} \frac{1}{g m_{air}} 10^{-6} \int_{0}^{P_{surf}} \chi'(P) dP$$

(4.19)

where $1/2.69e^{16}$ is the conversion factor from number of molecules per $m^2$ to DU, $g$ is the gravitational acceleration and $m_{air}$ is the mass of air. The profiles chosen in Figure 4.16 are the profiles for each period P1, P2 and P3 that give largest amplitude of ECMWF-deduced total ozone column perturbations in DU. The ECMWF-deduced total ozone column perturbations calculated for each of these profiles and thus the maximum ECMWF-deduced total ozone column fluctuations for each period are 0.95, 0.91 and 0.98 DU for respectively P1, P2 and P3. For the period P2 and P3 these maximum ECMWF-deduced fluctuations are consistent with observed fluctuations in the GOME total ozone columns of $\sim 1$ DU. The maximum GOME ozone column fluctuations in periods P2 and P3 are around 1.5 DU, a factor of 1.5 larger than the maximum ECMWF-deduced fluctuations. For P1 the discrepancy between maximum
**Figure 4.16:** Vertical distribution of calculated ozone perturbations in ppmv (top panels) and DU (lower panels) for three different date/longitude combinations: 27 August 1996, longitude=300° (figures a and d), 8 August 1998, longitude=125° (figures b and e) and 21 October 2000, longitude=120° (figures c and f).

ECMWF-deduced fluctuations and maximum GOME fluctuations is somewhat larger. The maximum ECMWF-deduced fluctuations for this period are a factor 2 smaller than the maximum GOME fluctuations of ~ 2 DU. We do see however that the amplitude of the ECMWF-deduced ozone fluctuations at 30 hPa is higher for P1 than for P2 and P3. An extended study using ozone profile measurements would be meaningful for the attribution of the cause of this discrepancy.

In Figure 4.18 we compare the phase of ECMWF-deduced ozone column fluctuations with the fluctuations previously identified in the GOME ozone columns in T04. The Figure shows longitude-time sections of the ECWMF-deduced total ozone column fluctuations for the three periods P1, P2 and P3. The added crosses indicate the timing and location of maximum GOME ozone column fluctuations (Note: the location of maximum GOME ozone column fluctuations may vary somewhat with the results in Figure 5 from T04. This is caused by the changed limits of the applied bandpass filter: 12 and 20 days compared to 10 and 15 days in T04. Furthermore, in contrary to this study, westward fluctuations have not been excluded in Figure 5 of
T04). There is a clear difference in timing of maximum fluctuations in both datasets. Also the wave periods of the GOME total ozone fluctuations seem somewhat shorter than those of the ECMWF-deduced ozone column fluctuations. These differences are an interesting outcome of this work, they might be related to a systematic error in the ECMWF data. Further study using additional datasources is needed to address the difference in timing and wave period.

Figure 4.19 shows the pressure versus time plots of the ECMWF-deduced ozone variations for the three periods P1, P2 and P3. Downward phase propagation can be seen. The phase changes sign above $\sim 10$ hPa caused by the sign change of the vertical gradient of mean ozone at this altitude. Amplitudes are maximum around 30 hPa as previously noted in Figure 4.16. The times of maximum and minimum GOME total ozone column fluctuations identified in T04 are respectively indicated by the solid and dashed vertical lines.

We have also explored another method to derive expected total ozone column variations, i.e. by using the linearised continuity equation

$$\frac{\partial u'}{\partial x} + \frac{\partial w'}{\partial z} = 0 \quad (4.20)$$

in combination with the linearised tracer continuity equation (4.15). The solution for $u'$ is given by equation (4.11). $u'(y)$ can be derived from the zonal wind fluctuations
4.5 Ozone column variations derived from ERA-40 u and T

Figure 4.18: Longitude-time section of GOME (upper 3 plots) and ECMWF-deduced (lower 3 plots) total ozone columns fluctuations for periods P1, P2 and P3. Solid lines start at zero DU with an increment of 0.5 for each contour line. Dashed lines start at -0.5 DU with a decrement of 0.5 DU for each contour line. Crosses denote phase maxima of GOME ozone column fluctuations.

found in the ERA-40 data. A drawback of this method is that the information contained in the ERA-data is only used to derive \( \tilde{u}(y) \), the information on the phase of the fluctuations in ERA-40 is not used. Furthermore the solution for \( u' \) and through equation (4.20) also for \( w' \) manifest an unrealistic exponential grow with altitude because of the \( e^{z\pi} \) factor. In reality the wave amplitudes will not grow exponentially with altitude, due to dissipation of the waves. These two factors make this method
Figure 4.19: Pressure versus time distribution of ECMWF-deduced ozone perturbations in DU for P1 at longitude=300° (upper plot), P2 at longitude=125° (center plot) and P3 at longitude=120° (lower plot). Solid contour lines start at zero DU with an increment of 0.2 for each contour line. Dotted contour lines start at -0.2 DU with a decrement of 0.2 for each contour line. Solid (dashed) vertical lines denote times of maximum (minimum) GOME ozone column variations at corresponding longitudes.
4.6 Conclusion and outlook

The ECMWF ERA-40 wind and temperature data provide information on the vertical structure of the Kelvin wave activity previously found in total ozone column data from GOME. Combined use of the ECMWF ERA-40 zonal wind and temperature fields and GOME total ozone column data offers the possibility to investigate the relation between Kelvin wave induced fluctuations in zonal wind, temperature and ozone concentrations.

Applying the bi-dimensional unequally spaced data spectral technique, introduced in T04, to the ERA-40 zonal wind and temperature data, revealed spectral features that are consistent with the spectral features found in the GOME ozone columns. The spectral features correspond to Kelvin waves with wavenumbers 1 and 2 and periods around 15-20 days and can be found between 100 and 10 hPa for all three high Kelvin wave activity periods identified in the GOME data (P1: 15 July to 13 September 1996, P2: 17 July to 15 September 1998 and P3: 19 September to 18 November 2000). The Kelvin wave induced perturbations are up to 8 m/s for the zonal wind and 2 K for the temperature. The vertical wavelength is 10-12 km. Calculations show that the perturbations in the temperature can lead to variations in the total ozone column of around 1 DU, which is consistent with the perturbations previously found in the GOME ozone columns for periods P2 and P3. For period P1 the calculated variations are about a factor 2 lower than observed. In these calculations we only took into account ozone fluctuations induced by horizontal and vertical transport. Ozone fluctuations induced by the temperature dependence of photochemical reactions that produce or destroy ozone are neglected, which is a good assumption in the lower part of the stratosphere. The Kelvin wave signals analysed in this study show characteristics of lower stratospheric Kelvin waves. In this region, neglecting photochemical effects on ozone is justified.

Higher up in the stratosphere the ozone fluctuations are photochemically controlled and the effect of transport on ozone is smaller [Salby et al., 1990, and references herein]. We could indeed see that the transport induced ozone fluctuations are largest below the ozone maximum, where the ozone gradient is largest, and become smaller above 40 km. The consistency between the calculated total ozone fluctuations from the zonal wind fluctuations indicates that the observed total ozone column fluctuations are indeed mainly caused by transport effects in the lower stratosphere.

In this study we used the zonal wind and temperature data to retrieve information on the vertical structure of the Kelvin wave signals found in the total ozone column measurements from GOME. For a more extensive and accurate determination of the vertical distribution of the Kelvin wave signals, we need ozone profile measurements with an adequate vertical resolution. Both ozone profiles derived from the GOME nadir measurements [Van der A. et al., 2002] and the SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) [Bovensmann et al., 1999] limb measurements will be analysed for this purpose in future work. The latter provides ozone profile data with a vertical resolution of ~ 3 km. The instrument per-
forms nadir column and limb profile measurements within 7 minutes of each other. The combination of these measurements will offer a good possibility for studying both the horizontal and vertical distribution of Kelvin wave activity.

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Equatorial Kelvin wave signatures in ozone profile measurements from GOME

abstract
This study investigates the ability to derive height resolved information on equatorial Kelvin wave activity from three different GOME ozone profile datasets. The ozone profiles derived using the Ozone Profile Retrieval Algorithm (OPERA) based on optimal estimation and the Neural Network Ozone Retrieval System (NNORSY), both show Kelvin wave signals in agreement with previously identified signals in the GOME total ozone columns. However, due to the inadequate vertical resolution, these two datasets are not able to resolve the vertical structure of the Kelvin wave activity. The third dataset, consisting of assimilated OPERA ozone profiles, does provide height resolved information on Kelvin wave activity that is in agreement with results from the analysis of GOME total ozone columns and ECMWF Re-Analysis (ERA-40) temperature data. Largest Kelvin wave induced perturbations of up to 0.69 DU/km coincide with the maximum vertical gradient in ozone around 35 hPa and show an in-phase relationship with temperature perturbations in ERA-40 as expected from theoretical considerations. These results indicate that the ozone perturbations in the lower stratosphere and in the total column of ozone are transport related. Between 10 and 1 hPa large Kelvin wave induced fluctuations in ozone mixing ratio are present that however, due to their small contribution to the total column, do not constitute a large contribution to the total ozone column perturbations. The ozone perturbations between 10 and 1 hPa show an out of phase relationship with temperature perturbations in ERA-40, indicating that the perturbations can either be caused by transport effects or photochemical influences.

5.1 Introduction
The equatorial Kelvin wave is one of the important types of waves present in the tropics. It is an eastward and vertically propagating wave. Because of its vertical propagation it can transport eastward momentum upward and thereby play a role in the driving of the quasi-biennial and semi-annual oscillations in the zonal wind.
In spite of their importance in the atmosphere, the climatology of equatorial Kelvin waves is still poorly known. Kelvin wave signatures have been detected in datasets from ground-based instruments [e.g. Wallace and Kousky, 1968; Hirota, 1978; Boehm and Verlinde, 2000; Holton et al., 2001]. A drawback of using ground-based measurements to investigate Kelvin waves is the lack of regularly operating stations around the equator, giving a poor horizontal coverage. Satellite measurements provide a mean to study the global distribution of Kelvin wave activity. Different satellite instruments have been used to study Kelvin wave signatures in either temperature or trace gas measurements [see e.g. Salby et al., 1990; Randel and Gille, 1991; Ziemke and Stanford, 1994; Canziani, 1999; Smith et al., 2002; Mote and Dunkerton, 2004]. However, the ability of these measurements to contribute to a global description of Kelvin wave activity is generally limited by either poor vertical resolution or the time period covered by available continuous datasets. In previous studies, Timmermans et al. [2004, 2005] (hereinafter T04 and T05) demonstrated the sensitivity of the GOME (Global Ozone Monitoring Experiment) ozone column measurements to Kelvin waves. In seven years of data, three periods of high Kelvin wave activity were found correlating with Kelvin wave signatures in ECMWF (European Centre for Medium-Range Weather Forecasts) Re-Analysis (ERA-40) data. The ERA-40 zonal wind and temperature data provide information on the vertical structure of the Kelvin wave activity found in the GOME total ozone columns.

To study the vertical distribution of the ozone fluctuations induced by Kelvin waves, ozone profile measurements are needed. In this study we investigate the vertical structure of the previously identified Kelvin waves by using ozone profiles measured by GOME. For this we will investigate three different datasets derived from the GOME measurements. The first consists of ozone profiles retrieved using the Ozone Profile Retrieval Algorithm (OPERA) based on optimal estimation [Van der A. et al., 2002; Van Oss and Spurr, 2002]. The second dataset consists of ozone profiles derived using the Neural Network Ozone Retrieval System (NNORSY) [Müller et al., 2003]. The third dataset consists of assimilated ozone profiles based on the above mentioned OPERA ozone profiles which are assimilated using the TM3 model driven by the ECMWF (ERA-40) meteorology [Segers et al., 2004]. The three datasets all have different characteristics concerning for instance accuracy and vertical resolution and will therefore give different results. The following section provides some details on the three datasets.

5.2 Data and analysis

5.2.1 GOME instrument

The GOME instrument was launched on 21 April 1995 on board the European Remote Sensing Satellite (ERS-2). It is a nadir-viewing spectrometer that measures the radiation of the sun that is scattered by the Earth’s atmosphere or reflected from the Earth’s surface. The measured radiation provides information on the ozone concentration in the atmosphere. The amount of absorbed radiation by ozone is depended on the wavelength of the radiation, e.g. radiation with a wavelength of 265 nm is more
strongly absorbed than radiation with a wavelength of 350 nm. Because of this, the 265 nm radiation from the sun will not reach the lower part of the atmosphere and only contain information on the upper layers of the atmosphere, while the 350 nm radiation will be able to pass through the entire atmosphere and contain information on the total ozone column. When going from 265 to 350 nm, the radiation will gradually reach deeper in the atmosphere and contain information on a larger vertical part of the atmosphere. The wavelength dependence of ozone absorption thus allows the derivation of information on the vertical distribution of ozone. The spatial resolution of the GOME ozone profile measurements is 100 km in latitudinal and 960 km in longitudinal direction. Global coverage is reached in three days.

5.2.2 OPERA O\textsubscript{3} profiles

The OPERA algorithm, used to derive the ozone profiles in this dataset, is based on the optimal estimation method, where information of the observation is combined with a-priori information. To get the best estimate the difference between observations and observations from a forward model as well as the difference between the a-priori information and the estimated parameters are minimised. The balance of these both contributions is determined using the observational errors and the errors in the a-priori values. The LIDORT (Linearized Discrete Ordinate Radiative Transfer) radiative transfer model is used to calculate the expected reflectance measured by the instrument, given a prescribed atmospheric composition. A-priori profiles are taken from an ozone climatology by Fortuin and Kelder [1998]. This is a zonal mean ozone climatology based on a 12 year observation period of ozone sonde stations and satellites. Due to the inclusion of an a-priori profile, the retrieved profiles is a mixture between true and the a-priori profile. The relation between retrieved profile $x_{\text{retrieved}}$, true profile $x_{\text{true}}$ and a-priori profile $x_{\text{apriori}}$ is given by:

$$x_{\text{retrieved}} = A(x_{\text{true}} - x_{\text{apriori}})$$  (5.1)

The averaging kernel is a measure for the limited ability of the retrieval to find the true profile. It relates the true anomaly (truth minus a-priori profile) to the retrieved anomaly (retrieval minus a-priori). The limited profile information in the spectral measurement appears in the averaging kernel as broad weighting functions indicating that the retrieved value at some altitude depends on the true profile in a certain vertical range around that altitude. The vertical extent of the averaging kernel can be viewed as the vertical resolution. A second feature of the averaging kernel is that it shows small values in regions for which there is little profile information in the measurement. This leads to a small retrieved anomaly in this region, or a retrieved value close to the a-priori. In other words, the optimal estimation retrieval tends to the a-priori in case the measurement contains little information.

The ozone profiles used in this study consist of 40 ozone column densities between 41 pressure levels between the surface and 0.1 hPa. The vertical resolution that can be resolved is about 5 km around the ozone maximum and poorer at other altitudes. For a more detailed description of the algorithm we refer to Van der A. et al. [2002]; Van Oss and Sparr [2002].
5.2.3 NNORSY O₃ profiles

Another approach to derive ozone profile information from GOME data is the use of neural networks, as is done with the Neural Network Ozone Retrieval system, NNORSY [Müller et al., 2003]. This approach assumes a mapping between the spectral data measured by GOME and the ozone profile, which can be approximated by a neural network R according to

\[ x = R(y, c, w) + \epsilon \]

(5.2)

where \( x \) is the ozone profile, \( y \) is the spectrum measured by GOME, \( c \) is a vector with supplementary input data, \( w \) contains the network model parameters, also called weights, and \( \epsilon \) is an error vector.

To find an optimal set of weights, the system has to be trained using a training dataset which consists of paired GOME spectral measurements and colocated ozone profile measurements from sondes and satellites. Once this is done, the neural network R can be applied to all observations.

Apart from spectral data, the network is fed with some geophysical parameters which include satellite and solar zenith angles, scan angle, pixel type (east, west or nadir), latitude and season, in-orbit time and a temperature profile from the UK meteorological Office (UKMO).

The NNORSY ozone profiles are estimated to have a vertical resolution of at best 3-5 km at geopotential heights of 15-32 km. For more details on this neural network approach we refer to Müller et al. [2003].

5.2.4 Assimilated OPERA O₃ profiles

Retrieved ozone profiles from GOME, which are described in section 5.2.2, are being assimilated in the 3D global chemistry-transport model TM3. One of the purposes is to get a better simulation of the vertical ozone distribution [Segers et al., 2004]. The transport model has been configured to simulate the global concentration of ozone on 44 levels up to 0.1 hPa. The horizontal resolution is 3° in longitude and 2° in latitude. The ozone chemistry is parameterized using a simple homogeneous chemistry (Cariolle scheme) and heterogeneous chemistry based on chlorine activation. The model is driven by the meteorological fields from the ECMWF.

The assimilation scheme is an extension of an existent assimilation scheme for total ozone columns. The scheme makes use of a three dimensional covariance model that accounts for the different correlation scales in ozone with respect to altitude and longitude. It also makes use of the averaging kernel information supplied with the O₃ profiles. For a more detailed description of the assimilation of GOME O₃ profiles, we refer to Segers et al. [2004].

5.2.5 Analysis method

For the detection of Kelvin wave signals in the ozone profiles, the same bi-dimensional spectral analysis method as applied in T04 and T05 has been used. The method has the advantages to be able to handle unequally spaced data and to allow easy determination of the significance of detected signals. It is an extended version of the
5.3 Results

1-dimensional Lomb periodogram [Press et al., 1992; Scargle, 1982] which allows the application to 2-dimensional datasets. Here we will apply the periodogram to each level separately, i.e. data as function of longitude and time. The periodogram values will give us an indication of the dominant frequencies in the dataset.

Before applying the periodogram, the OPERA and NNORSY O\textsubscript{3} profiles are regridded on a 5° × 5° grid. Furthermore three-day averages of the OPERA and NNORSY profiles are taken since GOME reaches global coverage in 3 days and 1 day averages would lead to numerous gaps in the dataset. The assimilated ozone profiles are provided daily with global coverage, so no time averaging has been applied. From all three datasets only the gridcells located at the equator are used in the analysis. We focus on this latitude band because Kelvin waves reach their maximum amplitude at the equator.

5.3 Results

In this section we will show results for the three different datasets for periods with high Kelvin wave activity. Period P1 (15 July to 13 September 1996) and P3 (19 September to 18 November 2000) correspond to the first and third of the three periods with high Kelvin wave activity previously identified in the total ozone columns from GOME [Timmermans et al., 2004].

5.3.1 OPERA O\textsubscript{3} profiles

Figure 5.1 (left panel) shows the periodogram values for P1 as function of wave period and pressure for eastward waves with zonal wavenumber 1 present in the OPERA ozone profile data. The maximum signal is found between about 10-50 hPa at wave periods of 15-20 days. This result agrees with the signal found in the GOME total ozone columns in T04. The right panel of Figure 5.1, which shows the periodogram of the integrated ozone profile as function of zonal wavenumber and wave period, agrees with the periodogram derived for the total ozone data (Figure 3.1, T04). The blue, green and red area respectively denote the 90%, 99% and 99.9% significant signals as explained in T04. The signal in the integrated profile shows a very good agreement with the signal in the ozone columns.

The left panel in Figure 5.2 shows a pressure versus longitude plot for the ozone perturbations on 23 August 1996 in P1, expected to be induced by Kelvin waves. To derive the perturbations that are expected to be induced by Kelvin waves the data are filtered as to preserve only the dominant wave frequencies found in the periodogram. The filter only retains zonal wavenumbers 1 and 2. In time a band-pass filter given by Murakami [1979] is applied with half amplitudes at 12 and 20 days. 23 August 1996 is chosen because maximum ozone perturbations within period P1 are found on this day. Note that it is also the day where maximum zonal wind perturbations in the ERA-40 data were found in T05. From this figure of filtered data, the tilt of the perturbations with height can be determined. Between approximately 7 and 100 hPa a wave 1 structure is visible with an eastward phase tilt with height, characteristic for eastward moving Kelvin waves. However the vertical extent of the positive and negative perturbations is too broad as can also be seen in the right panel of Figure
Figure 5.1: Left: Lomb periodogram for the OPERA ozone profiles, for zonal wavenumber 1 for the period 15 July to 13 September 1996. Right: Lomb periodogram for integrated OPERA ozone profiles for the period 15 July to 13 September 1996.

Figure 5.2: Left: Pressure versus longitude plot of waves 1 and 2 in the OPERA ozone profiles on 23 August 1996. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 DU/km with increments of 0.05 DU/km for each contour line. Dashed lines start at -0.05 DU/km with a decrement of 0.05 DU/km for each contour line. Right: Profile of the ozone perturbations on 23 August 1996 at longitude=85°.
5.2. Here we took a cross section of the pressure longitude plot at a longitude of 85°, the location where we found our maximum ozone perturbations. The positive perturbations extent over the entire vertical range where we see the wave 1 structure and in the profile of the perturbations we see only one large maximum around 20 hPa and no clear vertical wave structure. It seems like the vertical resolution of the retrieved profiles is insufficient to resolve the vertical wave structure of the Kelvin waves.

Although the vertical structure of the Kelvin waves is not completely resolved in our results for period P1, there is evidence of a Kelvin wave signal corresponding to the signal found in the GOME total ozone column data in T04. For period P3 this is not the case. While in the GOME ozone column data period P3 was identified as a period with high Kelvin activity, the OPERA ozone profiles do not show a clear Kelvin wave signal. Figure 5.3 (left panel) shows the periodogram values for P3 as function of wave period and pressure for eastward waves with zonal wavenumber 1 present in the OPERA ozone profile data. There is no maximum at the wave frequencies previously identified in the GOME ozone columns. The integrated ozone profile periodogram (Figure 5.3, right panel) does show a small signal at eastward propagating waves with wavenumber 1 and periods around 12 days, corresponding to the signal found in the GOME ozone columns. However this signal is not significant. This is supported by looking at the pressure versus longitude plot for the ozone perturbations on 27 October 2000 in P3 (Figure 5.4), expected to be induced by waves with Kelvin wave characteristics. There is no eastward but a westward phase tilt with height, which is in contradiction with Kelvin wave theory. Further investigation of the data will be needed to examine what is causing these unexpected results.
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Figure 5.4: Pressure versus longitude plot of waves 1 and 2 in the OPERA ozone profiles on 27 October 2000. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 DU/km with increments of 0.05 DU/km for each contour line. Dashed lines start at -0.05 DU/km with a decrement of 0.05 DU/km for each contour line.

5.3.2 NNORSY O$_3$ profiles

Figure 5.5 (left panel) shows the periodogram values for P1 as function of wave period and pressure for eastward waves with zonal wavenumber 1 present in the NNORSY ozone profile data. The maximum signal is found around 25 km at wave periods of 15 days in agreement with the signal found in the GOME total ozone columns in T04.

The left panel in Figure 5.6 shows a pressure versus longitude plot for the ozone perturbations on 29 August 1996 in P1, expected to be induced by Kelvin waves. As with the OPERA profiles the data are filtered for zonal wavenumbers 1 and 2 and in time a band-pass filter is applied with half amplitudes at 12 and 20 days. 29 August 1996 is the date within period P1 where we find largest ozone perturbations in the NNORSY data. Between approximately 20 and 30 km a wave 1 structure is visible with an eastward phase tilt with height, characteristic for eastward moving Kelvin waves. Again the vertical extent of the positive and negative perturbations seems too broad. The right panel of Figure 5.6 shows a cross section of the pressure longitude plot at a longitude of 160°, the location where we found our maximum ozone perturbations. No vertical wave structure can be seen, there is one large maximum around 25 km. As with the OPERA profiles the vertical resolution of the retrieved profiles seems insufficient to fully resolve the vertical wave structure of the Kelvin waves.

Similar to the results for the OPERA dataset, the NNORSY dataset also does not show a clear Kelvin wave signal in period P3. Figure 5.7 (left panel) shows the periodogram values for P3 as function of wave period and pressure for eastward waves with zonal wavenumber 1 present in the NNORSY ozone profile data. There is a maximum signal around 18 km and wave periods of 15 days, slightly larger than
5.3 Results

Figure 5.5: Left: Lomb periodogram for the NNORSY ozone profiles, for zonal wavenumber 1 for the period 15 July to 13 September 1996. Right: Lomb periodogram for integrated NNORSY ozone profiles for the period 15 July to 13 September 1996.

Figure 5.6: Left: Pressure versus longitude plot of waves 1 and 2 in the NNORSY ozone profiles on 29 August 1996. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 DU/km with increments of 0.05 DU/km for each contour line. Dashed lines start at -0.05 DU/km with a decrement of 0.05 DU/km for each contour line. Right: Profile of the ozone perturbations on 29 August 1996 at longitude=160°.
Figure 5.7: **Left:** Lomb periodogram for the NNORSY ozone profiles, for zonal wavenumber 1 for the period 19 September to 18 November 2000. **Right:** Lomb periodogram for integrated NNORSY ozone profiles for the period 19 September to 18 November 2000.

Figure 5.8: Pressure versus longitude plot of waves 1 and 2 in the NNORSY ozone profiles on 30 September 2000. A band-pass filter with half-amplitudes at 12 and 20 days has been applied. Solid lines start at 0 DU/km with increments of 0.05 DU/km for each contour line. Dashed lines start at -0.05 DU/km with a decrement of 0.05 DU/km for each contour line.

the wave periods of 12 days where we found the maximum signal in the GOME ozone column. The integrated ozone profile periodogram (Figure 5.7, right panel) does show maximum signal at eastward propagating waves with wavenumber 1 and
5.3 Results

periods around 12-15 days. However when looking at the pressure versus longitude plot for the ozone perturbations on 30 September 2000 in P3 (Figure 5.8), we do not see the eastward phase tilt with height that is characteristic for Kelvin waves.

5.3.3 Assimilated OPERA O$_3$ profiles

Figure 5.9 shows the periodogram values for P1 and P3 as function of wave period and pressure for eastward waves with zonal wavenumber 1 present in the assimilated OPERA ozone profile data. For P1 maxima can be seen around 5 and 40 hPa at wave periods of 15-20 days in agreement with the signal found in the GOME total ozone columns in T04. Another maximum for P1 is seen around 10 hPa at wave periods of 30 days. Because we calculate the periodogram values over 60-day periods, waves with periods of 30 days are the slowest waves we can detect, therefore the reliability of the detection close to 30 days is doubtful. For P3, maxima can be seen around 7 hPa and 30-40 hPa at wave periods of 15 days.

Figure 5.10 shows pressure versus longitude plots for the ozone perturbations on 13 August 1996 in P1 and 23 October 2000 in P3, expected to be induced by Kelvin waves. The same filters have been applied as with the previous two datasets. In this dataset 13 August 1996 and 23 October 2000 are the dates within the periods P1 and P3 where we find largest ozone perturbations in DU/km. In contrast with the results from the two previous datasets, here in both P1 and P3 a wave 1 structure is visible with the eastward phase tilt with height, characteristic for Kelvin waves. This structure is visible between ~ 20 and 70 hPa for P1 and between ~ 10 and 70 hPa for P3.
Kelvin waves in GOME ozone profiles

In Figure 5.11, cross sections of the pressure longitude plots at a longitude of 129° for P1 and 297° for P3, are shown. These are the locations where we found our maximum ozone perturbations. Maximum (negative) amplitudes of 0.65 DU/km and 0.42 DU/km are seen around 30-40 hPa, where the gradient in ozone is largest. These results are in agreement with previous studies [e.g. Kawamoto et al., 1997; Mote and Dunkerton, 2004]. Integrating the profiles of the ozone perturbations lead to maximum total ozone column perturbations of 1.2 DU in P1 and 1.9 DU in P3. These results compare well with the fluctuations found in the GOME total ozone columns of 1-2 DU.

In Figure 5.12 the same cross sections as in Figure 5.11 are shown but now the ozone fluctuations derived from the ERA-40 temperature fluctuations are shown. The calculation, which is explained in T05, is based on linear Kelvin wave theory and only includes transport effects. Photochemical effects on ozone are neglected. Ozone perturbations are then given by [Equation 9 in Salby et al., 1990]:

$$\chi' = \frac{\partial}{\partial z} S T'$$

(5.3)

where S is a background static stability parameter. Thus, when only considering transport effects, the induced ozone fluctuations are proportional to the vertical gradient in mean ozone and in phase with the temperature fluctuations for a positive vertical gradient of ozone. The altitude of the calculated maxima agrees very well with the altitude of the maxima in the assimilated OPERA data. The agreement between the maximum amplitude around 35 hPa of the calculated ozone fluctuations and the maximum amplitude of the ozone fluctuations in the assimilated OPERA is very good for period P3. For period P1, the maximum in calculated ozone fluctuations...
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Figure 5.11: Profiles of the ozone perturbations in the assimilated OPERA ozone profiles on 13 August 1996 at lon=129° (left plot) and 23 October 2000 at lon=297° (right plot).

Figure 5.12: Profiles of the ozone perturbations derived from the ERA-40 temperature perturbations on 13 August 1996 at lon=130° (left plot) and 23 October 2000 at lon=295° (right plot).

is slightly smaller than the maximum amplitude for the assimilated OPERA ozone. There are several possible reasons for this discrepancy, e.g. the vertical gradient in the ozone profile is larger than the values used in the calculation, the ozone fluctuations are not only caused by transport effects but also by photochemical effects, the temperature perturbations in the ERA-40 data are too small or the ozone fluctuations in
the assimilated OPERA data are too large. In the calculated ozone fluctuations we also see a large maximum around 80 hPa which is not reflected in the assimilated OPERA ozone fluctuations. A possible reason might be the lower vertical resolution and accuracy at lower altitudes of the OPERA ozone data that is assimilated.

Figure 5.13 shows the time evolution of the normalised ERA-40 temperature perturbations in combination with the normalised assimilated OPERA ozone mixing ratio perturbations at the altitude where we found maximum ozone perturbations. The two variables are nearly in phase for the 60-day period P1. However on 13 August 1996
where maximum ozone perturbations are seen, the temperature perturbations are not at their maximum yet. This might explain the discrepancy between the calculated ozone perturbations and the perturbations in the assimilated OPERA ozone. Contrarily on 23 October 2000 the ozone and temperature perturbations are in phase, supporting the good agreement between the maximum amplitudes on this date.

Figure 5.14 and 5.15 show pressure versus time plots of the ozone perturbations in P1 and P3, both in DU/km and ppmv. Large perturbations in the mixing ratio

Figure 5.14: Pressure versus time plots of the ozone perturbations for period P1 and lon=129° in DU/km (upper plot) and ppmv (lower plot). Solid contour lines start at 0 DU/km and 0 ppmv with increments of 0.1 DU/km and 0.05 ppmv for each contour line. Dashed lines start at -0.1 DU/km and -0.05 ppmv with a decrement of 0.1 DU/km and 0.05 ppmv for each contour line.
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Figure 5.15: Pressure versus time plots of the ozone perturbations for period P3 and lon=297° in DU/km (upper plot) and ppmv (lower plot). Solid contour lines start at 0 DU/km and 0 ppmv with increments of 0.1 DU/km and 0.05 ppmv for each contour line. Dashed lines start at -0.1 DU/km and -0.05 ppmv with a decrement of 0.1 DU/km and 0.05 ppmv for each contour line.

of ozone (ppmv) above 10 hPa can be seen that especially in P3 are out of phase with the perturbations below 10 hPa. This is probably caused by the change in sign of the vertical gradient of ozone. The perturbations above 10 hPa disappear when converting to DU and hence will not make a large contribution to the total ozone column perturbations.

As can be seen in Figure 5.16 these large ozone perturbations above 10 hPa are out of phase with ERA-40 temperature perturbations. Since the vertical gradient of ozone
5.3 Results

Figure 5.16: Normalised ERA-40 temperature (dashed line) and assimilated OPERA ozone (solid line) mixing ratio (ppmv) perturbations. Upper plot: for period P1 at 4.2 hPa and lon=125° for temperature and 123° for ozone. Lower plot: for period P3 at 5.2 hPa and lon=215° for temperature and 216° for ozone.

is negative at these altitudes, the ozone perturbations can be caused by transport effects following equation (5.3). At these altitudes however, photochemical influences on ozone can also start playing a role. Following Salby et al. [1990] ozone fluctuations will be photochemically controlled at altitudes above 4 hPa and consequently show an out of phase relationship with temperature perturbations.

The large perturbations above 10 hPa are not seen in the ozone perturbations
calculated from the ERA-40 temperature perturbations. An example of this is shown in Figure 5.17. Since the calculated values are based on transport effects only, it is possible that the ozone perturbations above 10 hPa are caused by photochemical effects. However also erroneous temperature fluctuations in the ERA-40 data or erroneous ozone perturbations in the assimilated OPERA data could be the cause of the discrepancy between the calculated and assimilated OPERA ozone perturbations above 10 hPa.

Figure 5.18 shows that the ERA-40 temperature perturbations for the same date and longitude as shown in Figure 5.17, have a large negative peak around 7 hPa. This is the altitude where we find the ozone maximum and hence the vertical gradient in ozone is small. Consequently, the calculated ozone perturbations through equation (5.3) are small. Above 7 hPa the temperature perturbations rapidly decrease, while the vertical gradient in ozone increases. A slightly higher altitude of the negative peak in temperature perturbations would lead to larger calculated ozone perturbations.

5.4 Conclusion and discussion

Three different sets of GOME ozone profile data have been studied to investigate the ability of retrieving information on Kelvin wave activity and its horizontal and vertical structure.

Two of the datasets (OPERA and NNORSY) do provide some information on Kelvin wave activity but cannot fully resolve the vertical structure of the Kelvin waves. They do, however, show that the Kelvin waves have their largest amplitudes between 20 and 30 km in agreement with theory. In these two datasets Kelvin wave
signals are present, in some cases weak, in agreement with signals previously identified in the GOME total ozone columns.

The third dataset, which consists of assimilated OPERA ozone profiles, is able to provide more height resolved information on the structure of identified Kelvin wave activity. Since the OPERA profiles do not contain this information, it must be originating from the ECMWF meteorological fields that are driving the assimilation model. The assimilated ozone profiles show variability that is in agreement with results previously found in the GOME ozone columns and ERA-40 temperature and zonal wind fields. The variability corresponds to eastward propagating waves with zonal wavenumbers 1 and 2 and wave periods between 12 and 20 days. The Kelvin wave induced ozone perturbations have amplitudes of up to 0.65 DU/km or 0.2 ppmv. Integrating these perturbations in the vertical give maximum total ozone columns perturbations of 1.2 to 1.9 DU, depending on the chosen period. These values are consistent with the maximum perturbations of 1-2 DU previously found in the GOME total ozone columns. The maximum ozone perturbations are found at the altitude where the vertical gradient in ozone is largest, around 35 hPa. At this altitude the ozone perturbations are nearly in phase with ERA-40 temperature perturbations, supporting the suggestion that these ozone perturbations in the lower stratosphere are induced by transport effects. The agreement between the ozone perturbations in the assimilated OPERA data and calculated ozone perturbations that are derived from the ERA-40 temperature perturbations, considering transport effects only, is good concerning the altitude and amplitude of maximum perturbations. Around 80 hPa the calculated ozone perturbations show large perturbations that are not resolved by the assimilated data, possibly due to the lower vertical resolution at these altitudes of the OPERA ozone profiles used in the assimilation.

Between 10 and 1 hPa large fluctuations in the ozone mixing ratio are present
that diminish in the conversion to DU. These higher altitude perturbations are out of phase with the ERA-40 temperature perturbations. Since the vertical gradient in ozone changes sign above 10 hPa, these perturbations could be induced by transport effects. However, at these altitudes photochemical influences on ozone can also start paying a role. Further investigation will be needed to be able to determine the source of the ozone perturbations above 10 hPa.

To be able to resolve fine vertical structure in ozone profiles, an adequate vertical resolution of the measurements is needed. The SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) instrument on board Envisat (ENVironmental SATellite), performs limb measurements of ozone with a vertical resolution of \(\sim 3\) km. In future, the combination of these measurements with the nadir measurements of the instrument providing total ozone columns is expected to form a unique mean for investigating both horizontal and vertical structure of the Kelvin wave activity.

**Acknowledgments.** The authors would like to acknowledge Ronald van der A and Arjo Segers from KNMI for the provision of OPERA ozone profiles and assimilated datasets and the support given for handling the data. We are also very grateful to Martin Müller (ZSW Stuttgart, now at NASA-GSFC) and his colleagues for providing the NNORSY ozone profiles.
Diabatic descent inside the polar vortices using long-lived tracers measured by satellite

6.1 Introduction

For satellite instruments with a limited latitudinal coverage, it is often difficult to find sufficient coinciding groundbased measurements for a thorough validation. Relaxing the geographical coincidence criteria might increase the number of colocations but especially in the case of strong horizontal gradients in the measured concentrations, this will not lead to a proper validation.

For the validation of the ILAS N$_2$O measurements, which have a very limited latitudal coverage, Bodeker et al. [2005] improved the number of coincidences by switching to a coordinate system based on potential vorticity. Since concentration isopleths of long-lived species tend to be closely aligned with potential vorticity contours, setting up coincidence criteria based on this coordinate system might be physically more appropriate than using common geographical coincidence criteria. To further increase opportunities for coincidences, the measurement grid can be filled using trajectory analyses. When doing this, corrections must be made to account for diabatic ascent and descent.

In this study we have inferred the diabatic descent and ascent rates, both inside and outside the polar vortices and in the vortex edge regions, from the time evolution of the long lived species nitrous oxide (N$_2$O). At high latitudes N$_2$O has a lifetime of 4 months (summer, 1000K) to 30 years (winter, 400K). N$_2$O only has tropospheric sources. From the troposphere the N$_2$O is transported into the stratosphere where about 95% is destroyed by photolysis. The N$_2$O concentration therefore decreases poleward and with altitude (see Figure 6.1).

For these calculations N$_2$O measurements made by the Improved Limb Atmospheric Spectrometer (ILAS), regridded to an equivalent latitude ($\phi_{eq}$), potential temperature ($\theta$) and time coordinate frame were used. Equivalent latitude is a potential vorticity based variable that allows easy separation of air masses inside and outside the polar vortex [Nash et al. 1996]. Section 6.3 gives a more detailed discussion on equivalent latitude and its use in validation studies.
Section 6.2 and 6.3 respectively describe the ILAS data used in this study and the regridding of the data to an equivalent latitude, potential temperature and time coordinate frame. In section 6.4 the different meteorological regimes for which the calculations were performed are defined. The method for determining the diabatic descent and ascent rates is explained in section 6.5 and the results from the calculations are presented in section 6.6. A discussion of these results is given in section 6.7. The calculated diabatic descent and ascent rates are used in trajectory calculations for extension of the ILAS data as outlined above and as presented in Bodeker et al. [2005]; Struthers et al. [2005]. Suggestions for their further use are given in section 6.8.
6.2 ILAS data

In this study Improved Limb Atmospheric Spectrometer (ILAS) version 5.20 measurements of N$_2$O are used. The ILAS instrument is described in section 1.4.2. The altitude range for the derived ILAS products is from cloud-top to ~ 60 km with a vertical resolution of about 2 km [Appendix in Hayashida et al., 2000]. The lowest altitude is sometimes limited due to a low signal from the sun (high absorption) through the lower atmosphere which disables the tracking of the sun by the instrument. The instantaneous field of view was 2 km wide for the visible spectrometer and 13 km wide for the IR spectrometer. The air density-weighted absorption of the solar radiation occurs over an effective path length of 200-300 km, so on average the sampling volume has a length of 250 km.

The ILAS version 5.20 N$_2$O measurements compare very well with validation measurements [Kanzawa et al., 2003]. The uncertainty of the N$_2$O measurements is better than 10% between 10 and 30 km. Between 30 and 40 km the uncertainty is larger than 50%. Above 40 km the total errors of the N$_2$O measurements are 200-360% which makes them unsuitable for most purposes. Taking into consideration the uncertainties and errors from Kanzawa et al. [2003], this study focuses on the altitude range between 10 and 40 km.

6.3 Regridding to (equivalent latitude,$\theta$,time) coordinates

When validating satellite measurements with ground-based measurements coincidence criteria are needed. In most cases these criteria are based on the geographical location of both measurements, e.g. the measurements must lie within 200 km distance of each other. Especially for occultation instruments with a small latitudinal coverage, such geographical coincidence criteria do not always provide sufficient coincidences between the satellite and the ground-based measurements for a proper validation. Furthermore geographical coincidence criteria do not take into account the possibility of strong zonal and meridional gradients in the concentration of the measured species. Because the concentration differences of long-lived tracers tend to be small along lines of constant potential vorticity, moving to a coordinate system based on potential vorticity should be advantageous for the comparison of ground-based and satellite measurements. Equivalent latitude is such a PV based variable, as will be explained in section 6.3.1. By shifting away from a longitude, latitude, altitude and time coordinate system to an equivalent latitude, potential temperature and time coordinate system, coincidences in equivalent latitude can be searched for, meaning that the air masses have the same potential vorticity. The shift in coordinate system also reduces the dimensionality of the coincidence criterion from 4 to 3 dimensions. Solar occultation measurements that may be limited in true latitude are likely to have a broader range in equivalent latitude and may therefore be coincident with some locations with which they were previously not coincident. This is illustrated in Figure 6.2 where the equivalent latitude of both the ILAS measurements and the ground-based station of Lauder, New Zealand, are plotted. Lauder is situated at a latitude of 45°S, which is not covered by the ILAS measurements (see Figure 1.8).
For the calculations of diabatic descent and ascent rates we used ILAS N$_2$O measurements regridded to an equivalent latitude, potential temperature and time coordinate frame.

6.3.1 Equivalent latitude

The equivalent latitude $\phi_{eq}$ is a potential vorticity variable defined as the latitude enclosing the same area as the associated PV contour [Nash et al., 1996]. It is a vortex aligned coordinate, with its maximum ($90^\circ$) at the center of the polar vortex. Two air masses on the same equivalent latitude line on an isentropic plane have the same potential vorticity so airmasses tend to move along constant equivalent latitude lines. There is a one-to-one relationship between equivalent latitude and PV. The form of this relationship is related to mixing processes on the isentropic level at which the PV is calculated. One location can have different equivalent latitudes at different potential temperatures/altitudes. At the vortex edge PV contours are close together (see Figure 6.3). Thus, moving poleward through the vortex edge the PV increases rapidly with a small increase of the area enclosed by the PV contours and hence a small increase in the equivalent latitude. In the midlatitudes the air is well mixed leading to a small increase of PV as function of equivalent latitude. Figure 6.4 shows an example of PV versus equivalent latitude demonstrating this principle.

In the vortex edge region the plot exhibits an "S" shape. An important advantage of switching to an equivalent latitude coordinate system is the easy determination of
6.3 Regridding to (equivalent latitude, $\theta$, time) coordinates

Figure 6.3: Potential vorticity at 450 K level on 2 October 2003 over the South Pole.

Figure 6.4: Potential vorticity on the 450K level on 2 October 2003 over the South Pole.

the vortex edge from this "S" shape. (see section 6.4).

6.3.2 Regridding algorithm

For the regridding of ILAS data to equivalent latitude, potential temperature and time we made use of daily PV fields (12 UTC, 2.5\(^\circ\) lat by 3.75\(^\circ\) long) from the UKMO
(United Kingdom Meteorological Office) on 21 potential temperature levels (see table 6.1), hereafter referred to as the analysis levels.

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<tr>
<th>Analysis level</th>
<th>Potential temperature (K)</th>
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<td>1</td>
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<td>1500</td>
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Table 6.1: Potential temperatures of the 21 analysis levels.

First, daily PV vs. equivalent latitude relationships are calculated on all 21 isentropic analysis levels from the UKMO PV fields. Subsequently the PV for each ILAS measurement is determined by linear interpolation in space and time of the UKMO fields. This requires first bi-linear interpolation of the UKMO data to the horizontal location of the ILAS measurement, then temporal linear interpolation of the UKMO data to the time of the ILAS measurement and finally vertical linear interpolation of the UKMO data to the potential temperature level of the ILAS measurement. We now have the PV at the location of the ILAS measurement. Then the equivalent latitude of the ILAS measurement is determined. This requires the vertical interpolation of the ILAS measurement onto an isentropic grid of 21 levels corresponding to the UKMO levels. Using the maps produced in the first step the equivalent latitude associated with this PV at the ILAS measurement location on that day and level is determined. The latitude and longitude coordinates of the ILAS measurement are now replaced by an equivalent latitude coordinate.
6.4 Meteorological regimes

The diabatic descent and ascent rates have been determined for 6 different meteorological regimes:

- Inside the Northern Hemisphere vortex
- Outside the Northern Hemisphere vortex
- Within the Northern Hemisphere vortex edge region
- Inside the Southern Hemisphere vortex
- Outside the Southern Hemisphere vortex
- Within the Southern Hemisphere vortex edge region.

Bodeker et al. [2005] divided the ILAS data into the 6 regions using the methodology of Nash et al. [1996]. In this method the potential vorticity is plotted against equivalent latitude. The PV distribution exhibits an "S" shape in the vortex region as shown in Figure 6.4. The determination of the vortex edge region is based on this distribution. The vortex edge is defined as the location with the highest PV gradient constrained with the presence of a reasonably strong westerly jet in the proximity of this location. The vortex edge region is defined as the area between the local minimum and maximum in the second derivative of PV versus equivalent latitude. The main advantages of this method compared to most other methods for determining the vortex edge and boundary region are the reduction of noise and analysis errors and the elimination of the need for choosing functional fits.

The vortex does not exist throughout the whole year. When there is no vortex in either the Northern or Southern hemisphere, no distinction is made in the concerned hemisphere between the vortex interior, exterior and edge region. In this period the diabatic descent and ascent rates are calculated for the whole hemisphere.

The dates of formation and break up of the vortex are determined by using the quantity $\kappa$, derived by Bodeker et al. [2002], which provides a measure of the strength of barriers to meridional transport. It combines the steepness of gradients in potential vorticity with the strength of the wind speed along potential vorticity isolines. To calculate the periods when the Arctic and Antarctic vortices where in existence, $\kappa$ values were calculated as a function of equivalent latitude for each day on each of the 21 analysis levels. Then, for each day, the maximum $\kappa$ values were extracted to provide time series of maximum $\kappa$ vs. day on each potential temperature surface. Whenever $\kappa$ was greater than 10% of maximum over the whole analysis period (1 November 1996 to 30 June 1997) the polar vortex was assumed to exist.

The diabatic descent and ascent rates have not been calculated during the 5 days before and 5 days after the vortex break up day. During the vortex break up, the $\text{N}_2\text{O}$ concentration changes rapidly because of mixing processes between the airmasses originating from inside and outside the vortex. In this period around the break up the changes in the $\text{N}_2\text{O}$ concentrations are not caused by diabatic movements and can therefore not be used for calculations of diabatic descent and ascent rates. As will be shown in section 6.5 and 6.7 we assume in our calculations that mixing is a minor
cause of \(N_2O\) concentration changes, which is clearly not true around the vortex break up.

The separation into meteorological regimes, for the 243 days when ILAS measurements are available, has been illustrated in Figure 6.5. Also indicated are the formation and break up of the vortex including the 10 days around vortex break up which are excluded in the calculations.

6.5 Determination of diabatic descent and ascent rates

To calculate the diabatic descent or ascent rates \(\frac{d\theta}{dt}\) we made use of the time evolution of the \(N_2O\) concentrations. Nitrous oxide (\(N_2O\)) belongs to the species with a relatively long lifetime. Concentration changes of long-lived species are mainly caused by dynamical processes because the timescale at which these processes take place are much smaller than the timescales of the chemical processes producing and destroying the long-lived species. By tracking a constant \(N_2O\) concentration in time one can infer the diabatic ascent or descent rates \(\frac{d\theta}{dt}\). This is illustrated in Figure 6.6. We assume that the concentration changes are only caused by diabatic movements and not by mixing of air from different equivalent latitudes (see section 6.7).

The calculations have been performed for the 6 meteorological regimes defined in the previous section and consist of the following steps.

- For each of the 243 days and 21 potential temperature analysis levels the regridded ILAS \(N_2O\) fields as function of equivalent latitude are read.
- In the presence of a vortex, for each of the measurement points we determine whether it lies inside or outside the vortex or in the vortex edge region.
- For all 6 meteorological regimes we calculate the mean \(N_2O\) distribution as function of potential temperature and daynumber. This is done by taking the average over all measurements on a specific day and analysis level that have an equivalent latitude falling inside the concerned regime. Note that in the absence of a vortex we take the mean over all measurements in the same hemisphere.
- The presence of multiple potential temperature levels with the same \(N_2O\) concentration may impede the tracking of constant \(N_2O\) concentrations. For our calculations we therefore need one potential temperature value matched to each \(N_2O\) value. To realise this, we fit a third order polynomial to the \(N_2O\) profiles calculated in the previous step. Figure 6.7 shows examples of such fits which are given by:

\[
\ln(\theta) = A + B[\ln(N_2O)] + C[\ln(N_2O)]^2 + D[\ln(N_2O)]^3
\]  

(6.1)

- For each meteorological regime we now track in time 21 isopleths of \(N_2O\) between 50 and 250 ppbv using the fitted \(N_2O\) profiles. \(N_2O\) profiles become very steep at higher altitudes where we find low (< 50 ppbv) concentrations, making our
Figure 6.5: Illustration of the meteorological regimes defined for the determination of the diabatic descent and ascent rates.
tracking method difficult and less reliable, therefore 50 ppbv is chosen as a lower limit for the tracked concentrations.

The tracking is done separately for periods where a vortex is present or not. For the given measurement period this gives us two periods in the Northern Hemisphere (before and after vortex break up) and three periods in the Southern Hemisphere (before and after vortex break up and after vortex formation). For each tracked isopleth in each meteorological regime and period this gives us a series of \((\theta, \text{day})\) pairs.

- To deal with spurious data points a Fourier series is fitted to the \((\theta, \text{day})\) pairs. Since it is expected that diabatic descent and ascent rates will vary smoothly with time and show an annual cycle, we use a combination of cyclic terms with a period of 1 year, i.e.:

\[
\theta = A + B \sin\left(\text{day} \cdot \frac{2\pi}{365}\right) + C \cos\left(\text{day} \cdot \frac{2\pi}{365}\right)
\]  

(6.2)

Taking the first derivative of these fits gives us smooth diabatic descent/ascent rates \((d\theta/dt)\) for each day and each \(\theta\) level.

6.6 Results

Figures 6.8 and 6.9 show the mean \(N_2O\) distribution as function of potential temperature and daynumber for the 6 meteorological regimes. The thick black lines denote the vortex breakup and in the Southern Hemisphere also the vortex formation. The 243 day time period does not include a vortex formation in the Northern Hemisphere.

After the vortex break up and before the formation of a new vortex we made no distinction between inside the vortex, outside the vortex and within the vortex edge.
As a result the N\textsubscript{2}O distribution is the same for all three regions in the hemisphere. Inside the vortex the N\textsubscript{2}O concentrations above 450-500 K are lower than outside the vortex because of diabatic cooling/descent of the airmasses inside the vortex region. The vortex edge acts like a barrier which prevents mixing with air from outside the vortex. When the vortex breaks up, the airmasses from inside and outside the vortex mix and the N\textsubscript{2}O concentration at high latitudes above 450-500 K rises quickly.

Figures 6.10 and 6.11 show the calculated diabatic descent and ascent rates for re-
Figure 6.8: Northern Hemisphere mean N₂O distributions (a) inside the Arctic polar vortex, (b) in the vortex edge region, and (c) outside the vortex. The black line denotes the calculated dates at each potential temperature surface for the Arctic vortex breakup. Beyond this date N₂O fields are not sorted with respect to the vortex and therefore the distributions during this period are identical in each panel.
Figure 6.9: Southern Hemisphere mean $N_2O$ distributions (a) inside the Antarctic polar vortex, (b) in the vortex edge region, and (c) outside the vortex. The leftmost black line denotes the calculated dates at each potential temperature surface for the Antarctic vortex breakup. The rightmost line denotes the dates for formation of the new vortex in 1997. Between these dates $N_2O$ fields are not sorted with respect to the vortex and therefore the distributions during this period are identical in each panel.
spectively the Northern and Southern hemisphere. The yellow and red colors indicate ascent (diabatic warming) and the green and blue colors indicate descent (diabatic cooling). We only tracked isopleths of N$_2$O larger 50 ppbv, therefore we do not get any values at higher altitudes. In the Southern Hemisphere the measurement period covers the formation of the polar vortex in April/May.

Figure 6.9 shows descending N$_2$O isopleths preceding the vortex formation, indicating diabatic descent. This diabatic descent is clearly visible in Figure 6.11 with values up to 8K per day. Following the vortex formation diabatic descent continues below the 700K potential temperature level. The values here are around 0.4-2 Kelvin per day. The presence of diabatic descent at all levels between February and June and the high descent rates at higher levels between February and April are in agreement to reports in Kawamoto et al. [2004]. Figure 6.12 (from Struthers et al. [2005]) compares the descent of three N$_2$O isopleths (0.04, 0.1 and 0.15 ppm) for the Southern polar vortex calculated by Kawamoto et al. [2004] and by our method. The descent rates (in km/month) are practically identical for the two methods. The small differences between both methods are caused by the different sampling of the ILAS data. Kawamoto et al. [2004] define Southern polar region as everything with an equivalent latitude smaller than $-70^\circ$ for the whole period of February to June. In the Northern Hemisphere, the measurement period does not cover the vortex formation, which prevents the identification of diabatic descent preceding the formation. In the presence of a vortex we see diabatic descent inside vortex from November to February, below the potential temperature level of 700-800 K. The descent in the NH is smaller than in the SH with values between 0 and 0.8 K/day. These results lie in the range of diabatic descent rates calculated in previous studies, compiled by Greenblatt et al. [2002]. After vortex breakup we see diabatic ascent rates of up to 1K/day.

### 6.7 Discussion

Our method to determine the diabatic descent and ascent rates by tracking a constant N$_2$O concentration in time assumes that local changes in N$_2$O concentrations are caused by diabatic movements only and mixing does not play a role. We assume that inside and outside the vortex meridional mixing is not a problem because there is no large gradient in tracer concentration, as can been in Figure 6.1. Conversely at the vortex edge there is a strong gradient. If strong mixing would take place between air parcels from inside and outside the vortex, this gradient would diminish. Therefore we assume that there is no mixing across the vortex edge. However, when the vortex breaks up there is strong mixing between air masses originating from inside and outside the vortex, therefore we exclude 5 days prior and 5 days after vortex break up in our calculations. In future we might diagnose the presence of anomalous mixing across the vortex edge by examining tracer relationships between N$_2$O and CH$_4$. These tracer relationships are disrupted by mixing of air parcels of different dynamical origin [Plumb and Ko, 1992; Plumb et al., 2000]. Mixing of air across the vortex edge will lower the tracer gradients at the vortex edge as is illustrated in Figure 6.13. Inside the vortex the isopleths move upward, outside the vortex the isopleths move down. This mixing would be detected in our method as diabatic ascent inside the vortex and diabatic descent outside the vortex. Hence if mixing would take place,
Figure 6.10: Diabatic descent and ascent rates as function of potential temperature and time for the three regions in the Northern Hemisphere: a) inside the polar vortex, b) in the polar vortex edge region and c) outside the polar vortex.
Figure 6.11: Diabatic descent and ascent rates as function of potential temperature and time for the three regions in the Southern Hemisphere: a) inside the polar vortex, b) in the polar vortex edge region and c) outside the polar vortex.
6.7 Discussion

Figure 6.12: Descent of three N$_2$O isopleths for the Southern polar vortex calculated by our method (dashed line) and the method of Kawamoto et al. [2004] (solid line). Grey lines denote the altitude in km.

Figure 6.13: Illustration of tracer structure before and after across vortex edge mixing. Black lines denote N$_2$O isopleths before mixing. Gray lines denote N$_2$O isopleths after mixing.
the inferred diabatic ascent rates inside the vortex are overestimated, while outside
the vortex they are underestimated. Contrarily inferred diabatic descent rates inside
the vortex are underestimated and outside the vortex are overestimated.

6.8 Outlook

The calculated diabatic descent and ascent rates can be used in non-isentropic trajec-
tory calculations to fill in the sparse ILAS data grids. From the ILAS measurement
points, backward and forward trajectories can be calculated. The species concen-
tration can then be added along the trajectory to the grid to increase the temporal
coverage of the ILAS data for validation studies.

Given a ground-based column measurement the equivalent latitude can be derived at
each theta level from the UKMO data. An ILAS profile of the species concentration
can be extracted from the grids. This profile can be integrated for direct compari-
son with the ground-based measurement. The trajectories will be almost along PV
isolines and thus close to straight lines along potential temperature and equivalent
latitude surfaces.

Where trajectories intersect original ILAS measurements, difference fields can be cal-
culated. These can be used for e.g. calculations of ozone loss rates inside the polar
vortices and examination of dehydration and denitrification inside the vortices. For
long-lived species the difference fields should be zero. If this is not the case the difference
fields provide an indication for the accuracy of the trajectories and the diabatic
descent and ascent rates used in the calculations of these trajectories.

The methods and techniques used in this study can also be applied to satellite mea-
surements other than from ILAS. The change to an equivalent latitude system which
allows easy separation into inside and outside the polar vortices, and the increase in
temporal and spatial coverage of the measurements through the use of trajectories is
expected to be useful for the interpretation and validation of other satellite measure-
ments. Calculations of diabatic descent and ascent rates are needed when performing
the non-isentropic trajectory calculations.

Acknowledgments. I would like to acknowledge the NIWA institute in Lauder and
especially Greg Bodeker for giving me the opportunity to visit their institute and helping
me to perform the work described in this chapter. I am also grateful to the ILAS project
and the U. K. Meteorological Office for providing the data for this study.
Summary and outlook

In this chapter a summary including conclusions is given of the work described in this thesis. At the end an outlook is given with suggestions for future research.

7.1 Summary

Below answers are provided to the four questions given in the introduction:

1. Can Kelvin waves be detected in total ozone column and ozone profile measurements from GOME?

2. Is the vertical resolution of the vertical ozone profiles from GOME sufficient to provide information on the vertical structure of the Kelvin wave activity?

3. How well do the Kelvin wave signals in the GOME measurements agree with Kelvin wave signals in temperature and wind data from the European Centre for Medium-Range Weather Forecasts (ECMWF)?

4. Can the diabatic descent or ascent rates in the polar vortices be determined from ILAS measurements of N$_2$O?

Question 1 has been addressed in chapters 3 and 5, question 2 in chapter 5, question 3 in chapter 4 and question 4 in chapter 6.

1. The variability of total ozone columns and profiles in the tropics measured by GOME, has been analysed by using a bi-dimensional spectral method. The method has been developed by extending an unequally spaced data technique first developed by Lomb from one to two dimensions. The method calculates which frequencies are dominant in a 60-day period and allows an easy determination of the statistical significance of an observed signal. In 7 years of GOME ozone column data three 60-day periods of high Kelvin wave activity are detected that correlate with westward equatorial zonal winds at 30 hPa: 15 July to 13 September 1996, 17 July to 15 September 1998 and 19 September to 18 November 2000. The three periods show significant signals at frequencies corresponding to eastward propagating waves with zonal wavenumbers 1 and 2 and wave periods of 12-15 days. The induced ozone perturbations of 1-2 DU can be attributed to ‘slow’ Kelvin waves in the lower stratosphere. Furthermore
three different datasets of GOME ozone profiles have been investigated: the OPERA ozone profiles derived using an algorithm based on optimal estimation, the NNORSY ozone profiles derived using a neural network and a dataset consisting of assimilated OPERA ozone profiles. All three datasets show Kelvin wave signals similar to those in the GOME ozone columns for the three high Kelvin wave activity periods identified in the GOME ozone columns.

2. Concerning the vertical distribution of the Kelvin wave activity, the OPERA and NNORSY ozone profiles provide some additional information compared to the GOME ozone columns. Due to their limited vertical resolution, both datasets cannot fully resolve the vertical structure of the Kelvin waves but do provide some height-resolved information. They show that the Kelvin wave induced ozone fluctuations have their largest amplitudes between 20 and 30 km, which is in agreement with theory. The assimilated OPERA ozone profiles that make use of a global chemistry-transport model driven by ECMWF meteorological fields show clearer height resolved information on the Kelvin wave activity identified in the GOME ozone columns. This information probably originates from the ECMWF meteorological fields and shows Kelvin wave characteristics that agree with other studies. Maximum Kelvin wave induced fluctuations with an amplitude of 0.65 DU/km (or 0.2 ppmv in mixing ratio) are found around 35 hPa, where the vertical gradient in ozone is largest. This is expected when the kelvin wave perturbations are induced by transport effects. The ozone mixing ratio also shows large Kelvin wave induced fluctuations between 10 and 1 hPa. These fluctuations diminish when making the conversion to DU and hence do not contribute largely to the total column perturbations. Vertical integration of the ozone perturbations leads to total ozone column perturbations between 1 and 2 DU in agreement with the perturbations in the GOME ozone columns.

3. ECMWF Re-analysis (ERA-40) fields of zonal wind and temperature are also analysed by using the same spectral method as is used for the GOME ozone measurements. For all three periods where the GOME total ozone columns display high Kelvin wave activity, the ECMWF fields manifest corresponding Kelvin wave activity. Spectral features associated with Kelvin waves of zonal wavenumber 1 and 2 and wave periods of 15-20 days are identified. The features are present between 100 and 10 hPa. The correlation between the Kelvin wave signals in the ECMWF fields and GOME ozone columns is good. The Kelvin wave induced perturbations in zonal wind and temperature are respectively up to 8 m/s and 2K. Assuming only transport effects play a role, these perturbations could lead to total ozone column perturbations of around 1 DU and maximum ozone perturbations around the height of maximum vertical gradient of ozone. This is in agreement with the results from the GOME ozone columns and assimilated OPERA data. The amplitude of the calculated maximum ozone perturbations also shows a good agreement with the amplitudes determined from the assimilated OPERA ozone profiles. The maximum ozone perturbations around 35 hPa in the assimilated ozone profiles are nearly in phase with the ERA-40 temperature perturbations. This indicates that the ozone perturbations in this altitude region are mainly caused by transport effects. The large ozone mixing ratio fluctuations between 10 and 1 hPa are out of phase with temperature perturbations. Further studies will be needed to investigate how large the contributions from trans-
7.2 Outlook

The vertical resolution of the GOME ozone profiles is too low to describe the vertical structure of the Kelvin wave activity. The SCIAMACHY instrument, on board Envisat, is performing nadir and limb measurements that will provide both total ozone columns and vertical profiles of ozone within 7 minutes of each other. The vertical resolution of these ozone profiles is around 3 km, which is expected to be sufficient for the detection of Kelvin wave structures with a vertical wavelength of around 8 to 10 km. The combination of nearly coinciding ozone columns and profiles will form a unique mean for the study of equatorial Kelvin waves. Additionally temperature profiles from the same platform, e.g. by GOMOS or MIPAS or from the ECMWF could complement the ozone data for studying the separate contributions of transport and photochemical effects to the Kelvin wave induced ozone perturbations. The identified perturbations in the GOME total ozone columns as well as around 35 hPa in the assimilated ozone profiles are attributed to transport by 'slow’ Kelvin waves in the lower stratosphere. The identified ozone perturbations between 10 and 1 hPa

port and photochemical effects are on these ozone perturbations.

4. Diabatic descent and ascent rates inside and outside the polar vortices have been inferred from the time evolution of N$_2$O measured by the ILAS instrument. The measurements cover the period of November 1996 to June 1997. Before the calculations are performed the data is regridded onto an equivalent latitude, potential temperature and time coordinate frame. Isopleths of N$_2$O are tracked to determine the descent or ascent rates inside, outside or at the edge of the polar vortices. In the Southern Hemisphere vortex strong diabatic descent is visible preceding the vortex formation with values up to 8 K per day. The descent continues inside the polar vortex after its formation with values around 0.4 to 2 K per day. The values are in agreement with other studies. In the Northern Hemisphere diabatic descent is visible inside the polar vortex below the potential temperature level of 700-800 K. The values are smaller than in the Southern Hemisphere, from 0 to 0.8 K per day, which lies in the range of values calculated in other studies. Following vortex break up diabatic ascent rates are seen with values up to 1 K per day.

Concluding, the work described in this thesis shows the potential of GOME measurements to contribute to a global description of Kelvin wave activity. The 3-dimensional structure can be analysed by using a combination with ERA-40 data or using assimilation of the GOME ozone profiles. Furthermore Kelvin wave signatures provide a tool to check the quality of the GOME ozone data in the tropics. This thesis also shows that satellite measurements of N$_2$O are a useful mean for the determination of diabatic descent and ascent rates. Overall the thesis demonstrates the ability of satellite measurements to improve the monitoring and understanding of dynamical processes in the atmosphere on a global scale.
however are probably originating from both transport and photochemical effects.

Kelvin waves play an important role in the equatorial atmosphere by their influence on the QBO and SAO. However the contribution of Kelvin waves to the forcing of these two large oscillations is still unclear and needs thorough investigation. Satellite measurements can contribute significantly to these investigations by providing information on the periods of large Kelvin wave activity, amplitudes and damping of the Kelvin waves.
Kelvin waves can also influence stratosphere-troposphere exchange. Combined use of satellite measurements and data from tropical stations could be used to investigate cross-tropopause transport, which deserves further study.

The calculated diabatic descent and ascent rates will be used in trajectory calculations, a.o. to fill in sparse ILAS data grids for validation studies. The method can also be applied to other satellite instruments, such as SCIAMACHY, MIPAS or MOPITT that measure long-lived trace species.
In our estimation of diabatic descent and ascent rates, it was assumed that mixing does not play a role in local changes in N$_2$O concentrations. To check the validity of this assumption the presence of anomalous mixing across the vortex edge can be examined by analysing tracer relationships between N$_2$O and CH$_4$.
The switch to an equivalent latitude system can be useful for several studies, especially for the separation of data from inside and outside the polar vortices and for increasing the number of coincidences between satellite and ground-based measurements in validation studies.
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References


# List of acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>ADEOS</td>
<td>ADvanced Earth Observing Satellite</td>
</tr>
<tr>
<td>CLAES</td>
<td>Cryogenic Limb Array Etalon Spectrometer</td>
</tr>
<tr>
<td>CRISTA</td>
<td>CRyogenic Infrared Spectrometers and Telescopes for the Atmosphere</td>
</tr>
<tr>
<td>DFT</td>
<td>Discrete Fourier Transformation</td>
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<tr>
<td>DOAS</td>
<td>Differential Optical Absorption Spectroscopy</td>
</tr>
<tr>
<td>DU</td>
<td>Dobson Unit</td>
</tr>
<tr>
<td>ECMWF</td>
<td>European Centre for Medium-range Weather Forecasts</td>
</tr>
<tr>
<td>ENVISAT</td>
<td>ENVironment SATellite</td>
</tr>
<tr>
<td>ERA</td>
<td>ECMWF Re-Analysis</td>
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<tr>
<td>ERS-2</td>
<td>second European Remote Sensing satellite</td>
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<tr>
<td>GDP</td>
<td>GOME Data Processing</td>
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<td>GOME</td>
<td>Global Ozone Monitoring Experiment</td>
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<td>GSFC</td>
<td>Goddard Space Flight Center</td>
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<tr>
<td>HALOE</td>
<td>HALogen Occultation Experiment</td>
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<tr>
<td>ILAS</td>
<td>Improved Limb Atmospheric Spectrometer</td>
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<tr>
<td>IR</td>
<td>Infra-Red</td>
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<tr>
<td>ISAMS</td>
<td>Improved Stratospheric And Mesospheric Sounder</td>
</tr>
<tr>
<td>KNMI</td>
<td>Koninklijk Nederlands Meteorologisch Instituut</td>
</tr>
<tr>
<td>LIDORT</td>
<td>Linearized Discrete Ordinate Radiative Transfer</td>
</tr>
<tr>
<td>LIMS</td>
<td>Limb Infrared Monitor of the Stratosphere</td>
</tr>
<tr>
<td>METOP</td>
<td>METeorological OPerational satellite</td>
</tr>
<tr>
<td>MLS</td>
<td>Microwave Limb Sounder</td>
</tr>
<tr>
<td>NCEP</td>
<td>National Centre for Environmental Prediction</td>
</tr>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
</tr>
<tr>
<td>NIWA</td>
<td>National Institute of Water and Atmospheric Research</td>
</tr>
<tr>
<td>NNORSY</td>
<td>Neural Network Ozone Retrieval SYstem</td>
</tr>
<tr>
<td>OPERA</td>
<td>Ozone ProfilE Retrieval Algorithm</td>
</tr>
<tr>
<td>POAM</td>
<td>Polar Ozone and Aerosol Measurements</td>
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<tr>
<td>PV</td>
<td>Potential Vorticity</td>
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<tr>
<td>QBO</td>
<td>Quasi-Biennial Oscillation</td>
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<tr>
<td>SAGE</td>
<td>Stratospheric Aerosol and Gas Experiment</td>
</tr>
<tr>
<td>SAO</td>
<td>Semi-Annual Oscillation</td>
</tr>
<tr>
<td>SBUV</td>
<td>Solar Backscatter UltraViolet instrument</td>
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<tr>
<td>SCIAMACHY</td>
<td>SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
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<tr>
<td>TIROS</td>
<td>Television and InfraRed Observation Satellite</td>
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<td>TOMS</td>
<td>Total Ozone Mapping Spectrometer</td>
</tr>
<tr>
<td>TOVS</td>
<td>TIROS Operational Vertical Sounder</td>
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<tr>
<td>UARS</td>
<td>Upper Atmosphere Research Satellite</td>
</tr>
<tr>
<td>UKMO</td>
<td>United Kingdom Meteorological Office</td>
</tr>
<tr>
<td>UTC</td>
<td>Coordinated Universal Time</td>
</tr>
<tr>
<td>ZSW</td>
<td>Center for Solar Energy and Hydrogen Research</td>
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Dankwoord

Het is zover! Mijn proefschrift is af. Het doel waar ik al die jaren naartoe heb gewerkt is bijna bereikt. Vreemd maar toch wel lekker. Het ging gepaard met de gebruikelijke hoogte- en dieptepunten, momenten dat alles lekker loopt maar ook momenten dat ik het even allemaal niet meer zag zitten en dat boekje onbereikbaar én ongewild lijkt. Gelukkig heb ik door de tijd heen steun gekregen van een hele hoop mensen. Met dit dankwoord wil ik graag al die mensen bedanken die mij op hun eigen manier geholpen hebben om mijn promotie goed door te komen.

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Ankie, zowel tijdens onze SCIAMACHY werkzaamheden als in de eerste periode van mijn promotie waarin je mijn begeleidster was, heb ik altijd heel fijn met je samen gewerkt. Je schijnbaar onuitputtelijke enthousiasme en energie werken motiverend en je vrolijkheid (slappe lach aanvallen) bracht vaak wat meer leven in de ietwat sombere SCIAMACHY brouwerij. Daarnaast ben ik je heel erg dankbaar voor de vrijheid die je mij in de laatste paar maanden hebt gegeven om me te concentreren op het afronden van mijn proefschrift. Dit betekende ongetwijfeld een zware last voor jou. Bedankt en veel succes verder met SCIA!

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