

Master's Thesis

**Broadband approach as a framework  
for implementation of radiative transfer scheme  
with selective intermittency:  
Cost versus accuracy study**

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2015

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# Chapter 1

## Basic Principles of Radiative Transfer

### 1.1 The Electromagnetic Spectrum

Radiation in the atmosphere is for the most part well represented by electromagnetic (EM) waves. Electromagnetic waves originate from multiple sources, most importantly the Sun, the Earth's surface and atmospheric gases and constituents (clouds and suspended particles). They have different wavelengths depending on the temperature of the radiating object through the Planck's law. Radiation of different wavelengths is subject to different levels of absorption and scattering when passing through the atmosphere. Traditionally, the electromagnetic spectrum is split into a number of regions (Fig. ??):

- Gamma radiation
- X-rays
- Ultraviolet radiation (UV-C, UV-B, UV-A)
- Visible light
- Infrared radiation (near IR, thermal IR, far IR)
- Microwaves
- Radio waves

Not all of them will be of our interest, because they are not represented in the atmosphere in energies high enough to influence its thermal structure. Specifically, our interest will be on everything between UV-C and far infrared.

### 1.1.1 Ultraviolet Radiation

Ultraviolet radiation (UV) is radiated in appreciable amounts only by very hot objects, such as the Sun. It is highly energetic, capable of causing electrons to be released from atoms (photoionisation) and breaking up molecules (photodissociation). Ultraviolet radiation spans wavelengths 10 – 400 nm. The UV spectrum is further split into multiple subregions, out of which only the last three are of interest to atmospheric radiative transmission<sup>1</sup>:

- UV-C: 100 nm–280 nm
- UV-B: 280 nm–320 nm
- UV-A: 320 nm–400 nm

Much of ultraviolet radiation is absorbed high in the atmosphere (stratosphere and mesosphere) by ozone and oxygen, though UV-A reaches the Earth's surface with little attenuation. Ultraviolet radiation has to be considered in radiation schemes, because it contributes significantly to heating of stratosphere. It is also important due to its influence on atmospheric chemistry (Chapman reactions).

### 1.1.2 Visible Light

The visible part of the spectrum comprises wavelengths which humans can perceive with their sight. The likely reason which gave rise to this ability is twofold. (1) This is where the peak power of Sun's radiation is located, and (2) the clear-sky atmosphere is almost transparent in the visible spectrum. Visible light spans the region of about 400 nm–700 nm. In radiation models it has to be considered due to its scattering and absorption by clouds and aerosols, but also due to relatively weak absorption by oxygen and ozone in a number of bands.

### 1.1.3 Infrared Radiation

Infrared radiation (IR) is emitted by objects of temperatures commonly found on Earth. Infrared spectrum can be split into three additional subregions:

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<sup>1</sup>The precise choice of boundaries is somewhat arbitrary, and various definitions can be found.

- Near infrared: 700 nm–4.6  $\mu$ m
- Thermal infrared: 4.6  $\mu$ m–50  $\mu$ m
- Far infrared: 50  $\mu$ m–1 mm

Radiation in near infrared comes mostly from the Sun, while standard temperature objects emit in the thermal and far infrared. The atmosphere is rather opaque to the infrared radiation. It is absorbed strongly (but not uniformly) by greenhouse gases: water vapour, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, CO, N<sub>2</sub>O~ and CFCs, but also by clouds and aerosols. As it is the main means of radiative energy exchange between the surface, atmospheric layers and space, it is of paramount importance to radiation models. Radiation in far infrared approx. above 100  $\mu$ m gradually ceases to be energetically important due to low power emitted at longer wavelengths.

#### 1.1.4 Shortwave and Longwave Spectrum

For the purpose of radiation models, it is convenient to adopt two even broader spectral regions – *shortwave* and *longwave* radiation. Though the choice of precise values is arbitrary, we will settle on the following definition:

- Shortwave radiation (UV, visible, near IR): 0–4.6  $\mu$ m
- Longwave radiation (thermal and far IR) : 4.6  $\mu$ m–100  $\mu$ m

The justification for this choice is that the Sun emits radiation mostly between 0.2–4.6  $\mu$ m, while the Earth's surface and atmosphere emit mostly at wavelengths longer than 4.6  $\mu$ m, with little overlap between the two (Fig. ??). As discussed later, this exceptionally lucky coincidence allows for decoupling of radiative transfer calculations in these two regions.

## 1.2 Fundamentals

This section summarises the basic theory of radiative transfer and notation used later in the text.



### 1.2.1 Frequency, Wavelength and Wavenumber

Frequency of a monochromatic EM wave will be denoted  $\tilde{\nu}$ . Frequency relates to wavelength  $\lambda$  via the speed of light  $c = \tilde{\nu}\lambda$ . Longer wavelengths are sometimes identified by wavenumber<sup>2</sup>  $\nu = 1/\lambda$ , esp. preferred in the infrared spectrum. It is notable that wavenumbers in  $\text{cm}^{-1}$  can be conveniently converted to wavelengths in  $\mu\text{m}$  by the expression  $y = 10000/x$ , where  $x$  is wavenumber and  $y$  wavelength (and vice-versa).

### 1.2.2 Radiance and Flux Density

Radiance<sup>3</sup> is power transmitted by an EM wave passing through a unit surface in a particular direction. Radiance is denoted as  $I_\lambda(\vec{r}, \vec{\Omega})$ , where  $\vec{r}$  and  $\vec{\Omega}$  determine the location and direction of interest (resp.). Radiance is sometimes denoted more specifically as *monochromatic radiance* to distinguish it from broadband radiance (integrated over wavelength). The units of radiance are  $\text{Wm}^{-2}\text{sr}^{-1}$ , and monochromatic radiance  $\text{Wm}^{-3}\text{sr}^{-1}$ .

Flux density  $F$  is radiance integrated over a hemisphere. In plane parallel geometry, depending on the hemisphere we speak of *upward* or *downward* flux density. Flux density integrated over surface is denoted simply as *flux*. Net flux density is flux density integrated over the full solid angle.

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<sup>2</sup>Symbols for frequency and wavenumber are sometimes reversed, with  $\tilde{\nu}$  denoting wavenumber, and  $\nu$  frequency.

<sup>3</sup>Radiance is sometimes referred to as *intensity*, *irradiance* or *exitance*. The latter two are reserved for radiance incoming on, and emitted from a surface (resp.).

### **1.2.3 Absorption Coefficient and Cross Section**

### **1.2.4 Emissivity and Albedo**

### **1.2.5 Optical Path and Transmissivity**

### **1.2.6 Heating Rate**

## **1.3 The Radiative Transfer Equation**

Fundamentally, radiative transfer is governed by the Maxwell equations and quantum mechanical principles. However, it is often not necessary to be concerned with the details of the electromagnetic field in the context of energy budget calculations, perhaps with the exception of Mie theory of scattering.

There are three energetically important processes in which radiation interacts with matter in the atmosphere: *scattering*, *absorption* and *emission*. Put together they form the radiative transfer equation.

### **1.3.1 Scattering**

Scattering of radiation occurs when a charged particle is made to oscillate in a passing electromagnetic wave, generating new electromagnetic radiation, which modifies the original field. There is no net exchange of energy between the particle and the field at the end of the process.

### **1.3.2 Absorption**

Passing radiation can be absorbed by molecules and particles, whereby the energy of a photon is absorbed to cause an electronic, vibrational or rotational transition (discussed later) in a molecule. This can be later turned into kinetic energy, causing an increase in temperature. The photon is lost in the process, and radiance is reduced by the corresponding amount of energy. The process of absorption follows quantum mechanical principles.

### 1.3.3 Emission

### 1.3.4 Beer's Law

### 1.3.5 Radiative Transfer Equation

The full form of the radiative transfer equation (RTE) combines the contributions of extinction, scattering, and emission in a single equation:

$$dI(\theta, \phi) = -\beta_e ds I(\theta, \phi) + \beta_s ds \int_{4\pi} I(\theta, \phi) p(\theta, \phi, \theta', \phi') d\theta' d\phi' + \beta_a ds B(\phi, \theta) \quad (1.1)$$

## 1.4 Solar Constant

The Sun emits radiation which closely matches that of black body of temperature about 5800 K. A fraction of the radiation reaches the top of the atmosphere (ToA). Because of the large distance of Earth from the Sun, the radiation can be considered parallel for most practical purposes. The solar flux density  $S$  at ToA in the direction of the Sun varies seasonally with Earth-Sun distance from about  $1330 \text{ Wm}^{-2}$  in July to  $1420 \text{ Wm}^{-2}$  in January (in contrast to seasons in the Northern Hemisphere). The solar flux density at mean distance is called *solar constant*, and denoted  $S_0$ . Solar constant is often cited to have value  $1366 \text{ Wm}^{-2}$ , though the exact value is time variable. One such variability is associated with the ~11-year solar cycle, but its amplitude is only about  $1 \text{ Wm}^{-2}$ . Longer-term variability also exists, but it is of little importance to NWP applications.

The solar constant and solar spectrum are best determined from space, where there is unhindered view of the Sun. There have been a number of such satellite-borne measurements performed over the past decades (Liou 2002).

## 1.5 Scattering on Spherical Particles

## Chapter 2

# Radiatively Active Gases

Radiation passing through the Earth's atmosphere is modified by the processes of absorption and scattering. Both of the processes are wavelength-dependent, but while scattering can be analysed by Rayleigh scattering, Mie theory and geometric optics, in order to fully grasp absorption we need to know the specific absorption lines of radiatively active gases.

Absorption functions of gas molecules can have immensely complicated structure. Figure ?? shows the absorption coefficient of CO<sub>2</sub> in various levels of magnification. Clearly, one needs a very large amount of information to describe the structure fully. As it turns out, smoothing the curve by averaging out the details is of little use in calculation of transmittance due to saturation at wavelengths where absorption is strongest (line centers). This will be discussed later, along with shortcuts to handle the situation efficiently.

[CO<sub>2</sub> absorption coefficient.]

### 2.1 Types of Transitions

Gases absorb and emit radiation at only precise wavelengths<sup>1</sup> due to restrictions imposed by the quantum theory. In particular, the energy has to match one of the allowed *electronic, vibrational* or *rotational* transitions.

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<sup>1</sup>But considering line broadening and continua discussed later in this chapter.

### 2.1.1 Electronic Transitions

Electronic transitions are the most energetic, associated with electrons transitioning into other energy levels within atoms, or breaking free entirely, in which case there is a continuum absorption, because any extra energy can transform into kinetic energy of the escaping electron. Electronic transitions are mostly responsible for absorption in the high-frequency part of the spectrum below 300 nm.

### 2.1.2 Vibrational Transitions

Vibrational transitions are less energetic than electronic, but more energetic than rotation transitions. They are due to transitions between vibrational modes of multi-atomic molecules. In quantum theory, they can be described by energy levels of a harmonic oscillator, having equally spaced levels obeying the equation

$$E_\nu = h\nu'(\nu + 1/2) \quad (2.1)$$

where  $\nu$  (Greek 'nu') is the *vibrational quantum number*. Not all molecules are capable of having vibrational transitions. They are subject to the condition that electromagnetic wave has to be able to exert force on the atoms, for which the molecule needs to have a dipole moment (be polarised). Notably, the most abundant atmospheric gas  $N_2$  does not have a dipole moment, and therefore does not possess vibrational modes<sup>2</sup>. The number of vibrational modes generally depend on the number of atoms in the molecule.

### 2.1.3 Rotational Transitions

Rotational transitions are caused by transitions between rotational modes of multi-atomic molecules. Rotational modes are quantised by the equation

$$E_J = \frac{1}{2I}L_J^2 = \frac{1}{2I}\left(\hbar\sqrt{J(J+1)}\right)^2 = \frac{\hbar^2}{2I}J(J+1) \quad (2.2)$$

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<sup>2</sup>However, vibrational transitions sometimes can occur even in these molecules if they are affected by EM wave at the time when there is a collision with another molecule of air, temporarily creating a dipole. Some molecules also form compounds in the form of dimers or multimers, in which case new modes may become available.

and the corresponding transitions between adjacent modes are

$$\Delta E = E_{J+1} - E_J = \frac{\hbar^2}{2I} [(J+1)(J+2) - J(J+1)] = \frac{\hbar^2}{I}(J+1) \quad (2.3)$$

where  $J$  is the *rotational quantum number* and  $I$  is moment of inertia of the molecule. Rotational transitions are the least energetic. As transitions can occur together, and because they are much less energetic than vibrational transitions, they combine to produce vibrational bands with fine structure, centered at a particular wavelength of a vibrational transition.

Not all molecules have rotational transitions. In particular, electromagnetic wave has to be able to exert torque on the molecule. Especially, it needs to have a dipole moment, or an intrinsic magnetic moment (as is the case with  $O_2$ ).

## 2.2 Shortwave Spectrum

In the shortwave spectrum, absorption takes place mostly in the high-frequency part of the spectrum (Fig. ??). In particular, gamma radiation, X-rays, UV-C and UV-B are almost entirely absorbed early in their travel through the atmosphere, mostly by oxygen and ozone. As such, and because they constitute only a small contribution of energy to low and mid-altitudes, they are of little concern to us. Above these wavelengths in the visible part of the spectrum, the atmosphere is relatively transparent, with only a few weak bands of ozone and oxygen. In near-infrared, radiation is again absorbed strongly by bands of water vapour and  $CO_2$ . This time we have to be concerned, because water vapour is mostly located in the troposphere, where it contributes to heating of atmospheric layers, and the absorption is not flat-out as in very short wave radiation.

### 2.2.1 O<sub>3</sub>

Ozone exhibits a number of bands in the shortwave spectrum in three groups: *Hartley bands*, *Huggins bands* and *Chappuis bands* (Figure 2.2.1). All of them are in the form of continuum due to photodissociation, although Huggins bands have more irregular structure.

Of the three, Hartley bands are the strongest. They cover the region between 240–310 nm. Because of their strength, they absorb most incident solar radiation in the mesosphere and stratosphere.

(Ozone shortwave bands. Data from Serdyuchenko et al. 2013, )(img/ozone-shortwave-bands.png)

Huggins bands cover the region of 310–340 nm.

Although Chappuis bands are the weakest of the three, they are important for atmospheric absorption, because they lie in the region of 450–750 nm, where solar radiation is the strongest. Their principal location of absorption is in the troposphere.

### 2.2.2 O<sub>2</sub>

Oxygen absorption happens mostly in the ultraviolet, where it is associated with electronic transitions.

Even though O<sub>2</sub> is a homonuclear diatomic molecule with no electric dipole moment, it has a permanent magnetic moment, enabling rotational transitions to occur.

Outside of the ultraviolet region, oxygen absorbs in the *red* and *infra-red* bands. They are associated with the  $a \leftarrow X$  (resp.  $b \leftarrow X$ ) electronic transition in combination with vibrational-rotational transitions. The red bands comprise band A centered at 762 nm, band B at 688 nm, and band  $\gamma$  at 628 nm. Infra-red bands are centered at 1.58  $\mu\text{m}$ , 1.27  $\mu\text{m}$  and 1.06  $\mu\text{m}$ . Although relatively sparse, the red bands are important to the tropospheric energy budget, because they are located at the peak of the solar spectrum (Liou 2002).

Oxygen molecules are known to form dimers with some other atmospheric constituents, notably O<sub>2</sub>.N<sub>2</sub> and O<sub>4</sub>. These have additional bands believed to contribute roughly 1 Wm<sup>-2</sup> to the total atmospheric absorption (Solomon et al. 1998).

## 2.3 Longwave Spectrum

### 2.3.1 Water Vapour

### 2.3.2 CO<sub>2</sub>

### 2.3.3 O<sub>3</sub>

### 2.3.4 Trace Gases

## 2.4 Distribution of Gases in the Atmosphere

## 2.5 Absorption Lines

Atmospheric gases do not in fact absorb and emit radiation at exact wavelengths – if they did we would probably hardly observe any absorption, because the likelihood of an EM wave of exact wavelength interacting with a molecule would be negligible. Instead, absorption lines are spread out over a range of frequencies by three types of processes:

- Natural broadening
- Doppler broadening
- Pressure broadening

*Natural broadening* occurs due to quantum mechanical effects and is very weak compared to the other two. Therefore, it has little importance to atmospheric radiative transfer.

*Doppler broadening* occurs due to Doppler shift in frequency as observed by a moving molecule. It has a normal (Gaussian) shape. Doppler broadening is relative strongest in the upper atmosphere.

*Pressure broadening* is the most important type of broadening to atmospheric physics. It occurs due to collisions between molecules, which impose a finite time limit on absorption and emission of a monochromatic EM wave.



Effects of all three types of broadening are combined together to produce a characteristic *line shape* of an absorption line. Line shape is defined as function  $f(\nu)$ , such that:

$$k_\nu = S f(\nu) \quad (2.4)$$

where  $S$  is the strength of a line. The shape function itself is normalised to unity:

$$\int_0^\infty f(\nu) d\nu = 1 \quad (2.5)$$

### 2.5.1 Pressure Broadening

Molecules in the atmosphere collide with each other at very high frequency. Every time a collision happens any absorption or emission process which is underway is interrupted. When a stimulation by a monochromatic wave is limited to a finite amount of time, this is equivalent to stimulation by a range of frequencies, which can be reconstructed by performing Fourier transform on the amplitude function. By taking into account the statistical distribution of time between collisions (Poisson distribution), we can calculate the relative probability of absorption/emission at every frequency. The derivation is carried out in e.g. Zdunkowski, Trautmann, and Bott (2007), here we show only the important result – the *Lorentz line shape*:

$$f(\nu) = \frac{\alpha}{\pi[(\nu - \nu_0)^2 + \alpha^2]} \quad (2.6)$$

where  $\nu_0$  is the line center and  $\alpha$  the line *half-width*. It should be noted that this only applies to high enough wavenumbers (compared to the half-width), but this is only concern to microwaves and longer wavelengths.

The half-width  $\alpha$  depends on the mean time between collision, which can be expressed in terms of pressure and temperature as:

$$\alpha = \alpha_0 \frac{p}{p_0} \left( \frac{T_0}{T} \right)^n \quad (2.7)$$

where  $\alpha_0$  is the half-width at reference pressure and temperature  $p_0$ ,  $T_0$ , and  $n$  is empirically determined exponent, which depends on the type of the molecule.

It has to be said that the theory outlined above (*Michelson-Lorentz theory*) does not hold exactly (Goody and Yung 1995). Especially, collisions themselves are not instantaneous, but take finite amount of time. Perhaps most importantly, the Lorentz line shape is insufficient in describing the line shape in far-wings of lines, which contribute very significantly to absorption in spectral windows, where there is no other absorption, and a far-wings of many distant lines add up. Overall, it has been established that the Lorentz line shape *underestimates* absorption in far-wings, and *overestimates* absorption near line centers.

### 2.5.2 Voigt Line Shape

### 2.5.3 Equivalent Width

The *equivalent width* of a line is the spectral width of a perfectly opaque square line which would absorb the same amount of radiation. For a line of any shape it can be calculated as:

$$W = \int_0^\infty (1 - e^{-k_\nu u}) d\nu \quad (2.8)$$

As such, it is not an intrinsic property of a line, but depends on the mass path  $u$ .

### 2.5.4 Weak Line Limit

It is useful to consider the special case when the amount of absorber is relatively small. The equation of equivalent width can then be linearised to give a simplified equation:

$$W = \int_0^\infty (1 - e^{-k_\nu u}) d\nu \approx \int_0^\infty (1 - (1 - k_\nu u)) d\nu = \int_0^\infty S f(\nu) u d\nu = Su \quad (2.9)$$

In the weak line limit, the absorption by a single line is independent from line shape, and it is linear with mass path.

### 2.5.5 Strong Line Limit

The equivalent width of an arbitrary Lorentz line is:

$$W = \int_0^\infty \left( 1 - \exp \left( - \frac{Su\alpha}{\pi[(\nu - \nu_0)^2 + \alpha^2]} \right) \right) d\nu \quad (2.10)$$

If the lower integration limit is extended to  $-\infty$ , and  $u$  is substituted by non-dimensional mass path  $\tilde{u} = Su/(2\pi\alpha)$ , the integration can be performed analytically to give:

$$W = 2\pi\alpha L(\tilde{u}) \quad (2.11)$$

where  $L$  is the Ladenburg-Reiche function, defined in terms of the modified Bessel function of the first kind:

$$L(\tilde{u}) = \tilde{u}e^{-\tilde{u}}[I_0(\tilde{u}) + I_1(\tilde{u})] \quad (2.12)$$

Using this analytical form, it can be shown that for large mass path, equivalent width approaches:

$$W \approx 2\sqrt{S\alpha u} \quad (2.13)$$

This is the *strong line limit*, when absorption by a single line grows in proportion to the square root of mass path  $\sqrt{u}$ .

The absorption by a single line starts off linearly, but with increasing absorber amount the monochromatic radiance near the line center becomes depleted, and the rate of absorption is reduced to sub-linear (square-root) regime. This can be thought of as *saturation* of absorption, and is similar in the context of multiple overlapping absorption lines.

## 2.6 Continuum

Gases absorb radiation in discrete absorption lines approximated by the Lorentz or Voigt line shape. However, in some molecules there are parts of the spectrum

where the absorption coefficient varies relatively little with wavelength, without apparent association with absorption lines. Typically, this *continuum absorption* occurs in connection with photoionization and photodissociation, when the extra energy is consumed by kinetic energy of the escaping electron, resp. broken-up molecules. These processes are mostly confined to the ultraviolet part of the spectrum, because of the high energies required. In addition to photoionisation and photodissociation, there are other less well- explained sources of continuum absorption at lower frequencies due to:

- Far-wings of absorption lines
- *Self continuum*
- *Foreign continuum*
- Absorption by dimers and multimers

Event though continuum absorption is generally weak comparable to line absorption (with the exception of UV) it is still of great importance, because it covers large parts of the spectrum, often in places where there is absence of line absorption (*atmospheric windows*).

### 2.6.1 Water Vapour Continuum

Water vapour is the most important source of continuum for the energy budget, responsible for as much as 40 % of longwave radiative cooling (Mlawer et al. [2012](#)). The continuum is mostly of two origins: far wings of lines and collision between molecules (self and foreign continuum).

### 2.6.2 Continua of Other Gases



## Chapter 3

# Approximate Solutions of the Radiative Transfer Equation

In order to make integration of the radiative transfer equation computationally feasible, and number of approximations are commonly taken along each axis of integration (spatial, zenithal/azimuthal, wavelength, time).

### 3.1 Plane Parallel Approximation

The atmosphere forms a thin envelope of the Earth with horizontal scales much pronounced relative to vertical scales. Factors influencing radiative transfer include gaseous concentrations, clouds, air and surface temperature variation. Perhaps with the exception of cumulus clouds, all of these change slowly in the horizontal direction, and we can simplify the calculations if we treat them as constant over relatively large areas. In NWP models, this is commonly done by dividing the computational domain into a grid and applying *plane parallel approximation* within each grid cell. In plane parallel approximation, the dependence of quantities on (x,y) coordinates is dropped, although dependence on zenithal and azimuthal angles can still be taken into consideration (e.g. via path length and diffusivity factor). Because plane parallel approximation leaves convective cloud structures unresolved, it is necessary to parametrise their influence by a special cloud overlap treatment.

Alternative to the plane parallel approximation is a full three-dimensional treat-

ment of radiation, generally performed by Monte Carlo simulation. This is however too computationally expensive to be done in today NWP models.

### 3.1.1 Layers

In the plane-parallel approximation the atmosphere is often discretized into *layers*, in which quantities such as temperature or gaseous concentrations are constant. Layer interfaces (boundaries) are defined by fixed vertical coordinates, usually pressure levels.

In the following text we assume that layers are numbered from top to bottom by integer number  $k$ , where  $k = 1$  is the uppermost layer, and  $k = N$  the layer just above the surface. Some quantities, such as fluxes, need to be determined on layer interfaces. The layer interface corresponding to the ToA will be numbered  $k = 0$ , increasing down to the atmosphere-surface interface  $k = N$ .

### 3.1.2 1-D Form of the Radiative Transfer Equation

The radiative transfer equation can be written in one dimensional form by defining  $\mu = |\cos(\theta)|$ , and noting that  $ds = dz/\mu$ :

$$\mu \frac{dI(\theta, \phi)}{dz} = -\beta_e I(\theta, \phi) + \beta_s \int_{4\pi} I(\theta, \phi) p(\theta, \phi, \theta', \phi') d\theta' d\phi' + \beta_a B(\phi, \theta) \quad (3.1)$$

## 3.2 Delta-Two Stream Approximation

In the  $\square$ -two stream approximation radiance is assumed to be constant over hemispheres, with the forward peak (from direct light sources) treated separately. Therefore, radiance is fully represented by two diffuse flux densities (upward and downward) and flux density of parallel radiation. The upward and downward diffuse flux densities will be denoted as  $F_{\uparrow}$  and  $F_{\downarrow}$ , and flux density of parallel (solar) radiation as  $S$ .

The  $\square$ -two stream approximation is justified by the fact that the scattering phase function of gases and atmospheric particles tends to be uniform with direction, with the exception of the forward peak. In Rayleigh scattering regime this holds

to great accuracy, while in the Mie regime the approximation is somewhat less sound.

### 3.2.1 Diffusivity Factor

### 3.2.2 RTE in Delta-Two Stream Approximation

The differential form of the RTE can be integrated over the azimuthal angle and both hemispheres to give two simplified ordinary differential equations valid for the two-stream approximation.

## 3.3 Band Models

Radiatively active gases usually have many more absorption lines than can be integrated over in NWP models in a time-effective manner. A number of statistical approaches to this problem have been invented. One well-established approach is *band models*, whereby line strengths are given by a statistical distribution specified by a limited number of parameters in each band (range of wavelengths). For suitably chosen distributions, the integration can be done analytically, leading to an expression for broadband transmissivity as a function of path length and distribution parameters. Traditionally, the band size has to be small enough that radiant power (Planck function) can be assumed constant within the band. With some effort this restriction can be lifted, at the cost of more complicating matters such as secondary saturation.

### 3.3.1 Malkmus Model

One of the most popular *narrow-band* models is the *Malkmus model*. It is based on the assumption that there is a given number of randomly distributed absorption lines in each band, and their strength has probability density:

$$p(S) = \frac{1}{S_0} e^{-S/S_0} \quad (3.2)$$

where  $S_0 = \int_0^\infty S p(S) dS$  is the mean line strength.



Optical depth at wavenumber  $\nu$  is the sum of contributions of all lines:

$$\tau = ku = \sum_{n=0}^N S_i u f(\nu) = \sum_{n=0}^N \frac{S_i u \alpha}{\pi[(\nu - \nu_i)^2 + \alpha^2]} \quad (3.3)$$

and narrow-band transmissivity

$$\mathcal{T} = \frac{1}{\Delta\nu} \int_{\nu_1}^{\nu_2} e^{-\tau} d\nu = \frac{1}{\Delta\nu} \int_{\nu_1}^{\nu_2} \exp\left(-\sum_{n=0}^N \frac{S_i u \alpha}{\pi[(\nu - \nu_i)^2 + \alpha^2]}\right) d\nu \quad (3.4)$$

The above expression is a random variable (because  $S_i$  and  $\nu_i$  are random variables). Therefore, we have to compute mean transmissivity to be useful:

$$\bar{\mathcal{T}} = \int_{\mathbf{S}} \int_{\nu} \mathcal{T} p(\nu) p(\mathbf{S}) d\nu d\mathbf{S} \quad (3.5)$$

where  $\mathbf{S} = (S_1, \dots, S_N)$  and  $\nu = (\nu_1, \dots, \nu_N)$  are vectors of line strengths and line positions. This integration can be performed analytically (see e.g. Zdunkowski, Trautmann, and Bott 2007), leading to the *Malkmus formula* for optical depth:

$$\tau_M = -\frac{\pi\alpha}{2\delta} \left( \sqrt{1 + \frac{4\bar{S}u}{\pi\alpha}} - 1 \right) \quad (3.6)$$

This formula can be adapted to the case of non-uniform line width  $\alpha$  by comparing two limiting cases of small and large mass paths to the weak and strong line limits derived in Sec. ?. The formula is first written in terms of parameters  $a$  and  $b$ :

$$\tau_M = -\frac{a}{2b} \left( \sqrt{1 + 4bu} - 1 \right) \quad (3.7)$$

By making approximations for  $4bu \ll 1$  and  $4bu \gg 1$  match the weak and strong line limits, one can show that

$$a = \sum S_i \quad (3.8)$$

$$b = a^2 / \left( \sum 2\sqrt{S_i \alpha_i} \right)^2 \quad (3.9)$$

### 3.3.2 Curtis-Godson Approximation

The Malkmus formula has a number of drawbacks. One of the more serious is that the line width  $\eta$  is assumed to be constant over the path. In reality, we often need to compute transmissivity over large parts of the atmosphere, where  $\eta$  varies with pressure and temperature due to line broadening. This situation is handled by the *Curtis-Godson approximation* for inhomogeneous atmospheres.

## 3.4 k-distribution Method

## 3.5 Continuum

### 3.5.1 MT\_CKD

Perhaps the most comprehensive model of continuum absorption is MT\_CKD produced by AER (Mlawer et al. 2012). It includes continuum absorption by water vapor, nitrogen, oxygen, carbon dioxide and ozone. The model uses a semi-empirical approach in which theoretical impact line shape modified by a  $\eta$ -function is fitted by measured values.

## 3.6 Adding Method

The *adding method* is a method of finding a solution to fluxes for given optical depths and temperature of layers. The adding method assumes that the plane parallel approximation,  $\eta$ -two stream approximation and layer discretization have been made.

A relationship between fluxes at the top and bottom interfaces of a layer can be found from the  $\eta$ -two-stream differential equations.

$$\begin{pmatrix} S_k \\ F_k^\downarrow \\ F_{k-1}^\uparrow \end{pmatrix} = \begin{pmatrix} a_1 & 0 & 0 \\ a_2 & a_3 & a_4 \\ a_5 & a_6 & a_7 \end{pmatrix} \begin{pmatrix} S_{k-1} \\ F_{k-1}^\downarrow \\ F_k^\uparrow \end{pmatrix} \quad (3.10)$$

The equations for all layers can be consolidated into a system of linear equations:

$$\mathbb{A}\mathbf{F} = \mathbf{S} \quad (3.11)$$

where  $\mathbb{A}$  is a matrix of coefficients (layer transmissivities and reflectivities),  $\mathbf{F}$  is a vector of fluxes and  $\mathbf{S}$  is a vector of sources. This system can then be solved for  $\mathbf{F}$ , which is the desired outcome of the adding method.

### 3.7 Net Exchange Rate

### 3.8 Time Intermittence

Because the temporal variability of all quantities coming as an input to the RTE is not the same, it is convenient to avoid repeated computation of certain results. E.g., the rate of change of cloudiness is much higher than that of gas concentrations. Therefore, it is possible skip or linearise the computation of gaseous transmission functions. Other intermediate results may also be reused, depending on the actual implementation of the solution.

## Chapter 4

### ACRANEB

ACRANEB (Ritter and Geleyn 1992) is a radiation scheme developed as an alternative to RRTM (Rapid Radiative Transfer Model) for use in NWP models. In contrast to k-distribution method employed by RRTM, ACRANEB uses a broadband model in only two spectral regions – shortwave and longwave, along with combined adding method/net exchange rate approach to finding spatial solution of the radiative transfer equation. Decrease in accuracy is compensated by more frequent updating of cloud cover made possible by shorter integration time.

ACRANEB is currently used operatively as a module in the NWP model ALARO by a number of countries.

#### 4.1 Operation Overview

The ACRANEB scheme is run on a single cell of the model computational grid. Vertically, the atmosphere is split into layers, on which the computation is discretized. In the ALARO model, the layers are defined in hybrid *eta* coordinates, transitioning smoothly from  $\sigma$ -coordinates near the surface to pressure coordinates in the free atmosphere. Therefore, boundary layers follow the ground, while upper layers follow isobaric surfaces.

The input to the radiation scheme consists of:

- Pressure profile

- Temperature profile
- Concentration of gases
- Cloud fraction and cloud water/ice content
- Aerosol fraction and properties (?)
- Surface temperature and albedo/emissivity
- Solar constant (?)

The output of the scheme are the broadband fluxes at layer interfaces, from which the heating rate of layers can be calculated.

Apart from an NWP model, ACRANEB can be run in isolation inside a single-cell model. This is useful mostly for diagnostic purposes.

## 4.2 Broadband Regions

The ACRANEB scheme operates in two spectral regions:

- Shortwave: 245 nm – 4.642  $\mu$ m
- Longwave: 4.642  $\mu$ m – 105.000  $\mu$ m

In the shortwave region, there is a single source of radiation (the Sun, resp. Moon), which undergoes scattering and absorption in every layer.

In the longwave region, the surface and every layer is a source of radiation through thermal emission, but this complexity is somewhat reduced by the fact that scattering of infrared radiation by gases in the atmosphere is weak enough to be neglected, although scattering of infrared radiation by clouds and aerosols still needs to be taken into account.

## 4.3 Gaseous Transmission

The radiation model depends on the ability to calculate gaseous transmission function between arbitrary layers. Transmission functions are approximated by a *modified Malkmus model*. The complex absorption structure of a gas is parametrised by a small number of parameters as it is in the classical narrow-band Malkmus model,

but in this case they describe the whole broadband region (shortwave or longwave). This greatly reduces the number of calculations needed to compute a transmission function between two layers, but necessitate a range of compromises to be made.

#### 4.3.1 Modified Malkmus Model

The modified Malkmus model is given by a heuristically derived formula based on the original Malkmus formula (Mašek, Král, and Brožková 2012):

$$\tau_M = \frac{a}{2b} \left( \sqrt{1 + \frac{4bu}{1 - c/a}} - 1 \right) \quad (4.1)$$

$$\tau = \frac{\tau_0}{\alpha} \left[ \left( 1 + \frac{\tau_M}{\tau_0} \right)^\alpha - 1 \right] \quad (4.2)$$

Coefficients  $a$ ,  $b$ , and  $c$  depend on pressure and temperature by:

$$a = a_0(T/T_0)^{\alpha_a}, b = b_0(p_0/p)(T/T_0)^{\alpha_b}, c = c_0(p/p_0)(T/T_0)^{\alpha_c} \quad (4.3)$$

The parameters  $a_0$ ,  $b_0$ ,  $c_0$ ,  $\alpha_a$ ,  $\alpha_b$ ,  $\alpha_c$ ,  $\alpha$  and  $\alpha_0$  are determined by fitting the transmission function to a range of transmissions calculated by an external narrow-band model SPLIDACO.

#### 4.3.2 Representation of Gases in ACRANEB

ACRANEB contain representation of all atmospheric gases which contribute significantly to the radiative energy budget in shortwave and longwave part of the spectrum:

- Water vapour
- O<sub>3</sub>
- CO<sub>2</sub>+ (CO<sub>2</sub>, CH<sub>4</sub>, CO, N<sub>2</sub>O, O<sub>2</sub>)

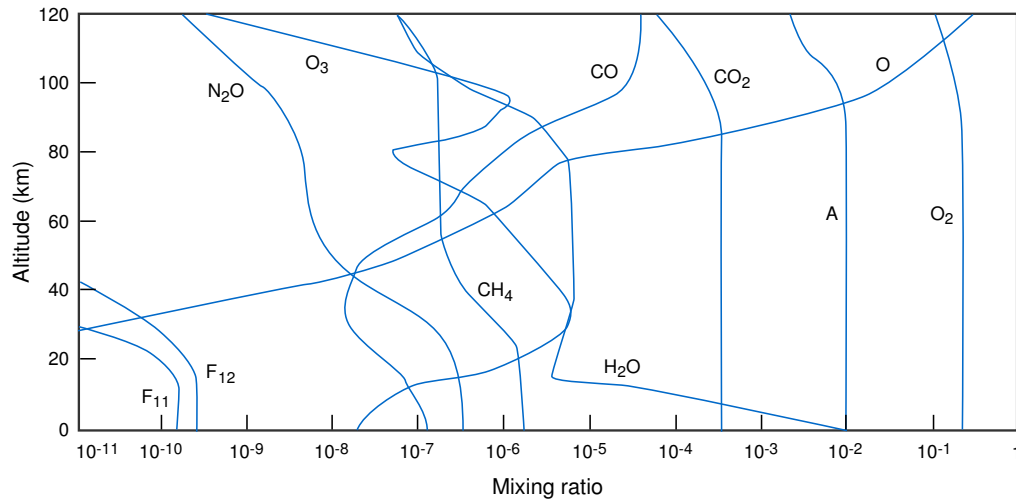


Figure 4.1: **Atmospheric composition.** Schematic figure showing concentration of some radiatively active gases in the atmosphere. Adapted from Goody and Yung 1989.

$\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{N}_2\text{O}$  and  $\text{O}_2$  are treated as a single *composite gas* (' $\text{CO}_2^+$ '), because they are well-mixed, and their concentration in the atmosphere is relatively constant<sup>1</sup> (Fig. ??).

The absorption structure of each gas is described by a total of 16 parameters (8 for both parts of the spectrum), as detailed above.

## 4.4 Solving the RTE

The solution for broadband flux densities at layer interfaces is found by multiple passes of the adding method outlined in the previous chapter. The adding method allows for only single absorption and scattering coefficient to be specified per layer. While this is sufficient for monochromatic calculations when the absorption and scattering coefficients are independent from the flux density, in

<sup>1</sup>This is not necessarily true for all conditions, because some of these gases have sources near the surface, e.g.  $\text{CO}_2$  is released by vegetation and exhibits both spatial and seasonal variability. Nevertheless, this simplification is justified, because the impact on atmospheric heating rate is low [citation?].

broadband calculations the power distribution of the flux needs to be taken into account. This is however not possible when fluxes combine contributions from multiple sources, with radiation having traversed different paths through the atmosphere.

One solution to the problem would be to carry out the adding method for every radiation source independently, and summing up the resulting fluxes (which can be done thanks to linearity of the RTE). The power distribution of a broadband flux at a layer interface can then be known, because it is determined by the power distribution of the emitting source and the extinction along the path between the source and the layer. To be precise, the path traversed by radiation between the source and the layer is not known with full accuracy, because apart from the direct path, a fraction of the radiation can be scattered multiple times, taking a longer path before arriving at the layer.

While the method outlined above is feasible and relatively accurate, it is too computationally demanding to be performed at every time step, because the adding method would have to be repeated for each layer in the thermal spectrum (every layer is a source of radiation). The number of passes can be reduced when we consider the net exchange rate formulation:

i.e. when we compute the flux divergence  $R_k$  by the adding method, it is equal to the sum of CTS, EWS and EBL terms. For a suitable choice of sources,

## 4.5 Net Exchange Rate Formulation

The adding method introduced in the previous chapter can be used to calculate fluxes at layer interfaces when source terms (sources of radiation) and optical depths of layers are known. However, this approach cannot be used directly for broadband calculations. This is because the optical depths are dependent on the actual power distribution with wavelength in affected flux, i.e. certain wavelengths can be selectively depleted by previous absorption, and further absorption becomes saturated (non-linear). Because there is only one broadband flux incorporation contributions of many sources, there is no way of specifying single right optical depth of a layer in the adding method equation. But this does not preclude the possibility to find one that is the most optimal.

An important observation about the radiative transfer problems is that it is linear – the radiative transfer equation can be solved separately for each radiation source,



and total radiances (or fluxes) can be obtained by summing the elemental solutions. Therefore, in theory, the adding method can be applied for each radiation source only, ensuring that layer optical depths can be chosen (almost) unequivocally, because the path between the layer and source is well known. The only exception is multiple scattering, when the path is prolonged, but this may be a relatively negligible effect. This method however cannot be employed efficiently in radiative transfer models, because there are too many sources (in the longwave spectrum every layer is a source). But some sources are more important than others – radiation exchange with surface and space are generally stronger than exchanges between layers. The space is not a radiation source (rather a ‘sink’), but the situation can be mathematically inverted to treat it as a source instead.

ACRANEB, being a broadband radiative model, has to make a number of simplifying assumptions in order to be able to leverage the adding method.

#### **4.5.1 Statistical Model**

#### **4.5.2 Autoevaluation**

### **4.6 Verification**

ACRANEB belongs to the category of less accurate but fast radiative transfer models. As such, it can use RRTM or LBL models as a verification target.

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