Discrete ordinate method

Single scattering properties

Molecular absorption

Radiative transfer

- 1 Radiation
 - What is radiation?
 - Radiance I and irradiance E
 - Blackbody radiation
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 - Derivation
 - Direct-diffuse splitting of radiation field
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 - Solution of RTE using the DOM
 - DOM Impact of number of streams
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What is radiation?

Two pictures:

- electromagnetic waves that propagate with speed of light (c = 2.998.10⁸ m/s)
- photons having zero mass and energy E=hν (Planck constant h = 6.626·10⁻³⁴ Js, frequency ν [1/s])

The wavelength λ of the radiation can be obtained from the relation

$$\boldsymbol{c} = \lambda \cdot \boldsymbol{\nu}$$

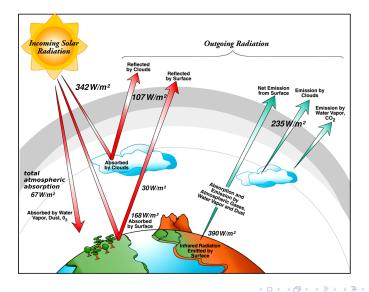
Radiative transfer equation

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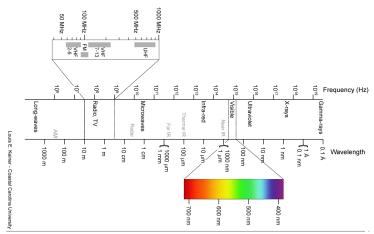
Radiation balance of the Earth



Single scattering properties

Molecular absorption

Electromagnetic spectrum



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ation Radiative transfer equation

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Radiance I and irradiance E

• Radiance L_{ν} :

 $\mathrm{d} \mathbf{Q}_{\nu} = \mathbf{I}_{\nu} \cos \theta \mathrm{d} \nu \mathrm{d} \sigma \mathrm{d} \omega \mathrm{d} t$

Unit: W/(m² Hz sr) or W/(m² nm sr)

• Irradiance E_{ν} :

$${\it E}_{
u} = \int {\it I}_{
u} \cos heta {
m d} \omega$$

Unit: W/(m² Hz) or W/(m² nm)

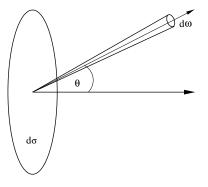


Figure: Definition of radiance.

Radiation

Discrete ordinate method

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Molecular absorption

Blackbody radiation

Planck function

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp\left(\frac{h\nu}{k_{\rm B}T}\right) - 1}$$

Unit: W/(m² Hz sr)

• Wien's displacement law (Maximum of Planck function)

$$\lambda_m = \frac{2897}{T}$$

• Stefan-Boltzmann's law (integrated Planck function)

$$E = \sigma_{\rm SB} T^4$$

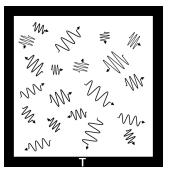


Figure: An opaque container at absolute temperature T encloses a "gas" of photons emitted by its walls. At equilibrium, the distribution of photon energies is determined solely by this temperature. The distribution function is called *Planck (distribution) function* (Figure from Bohren and Clothiaux, 2006)

Radiation	Radiative	transfer	equa
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Discrete ordinate method

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Planck radiation

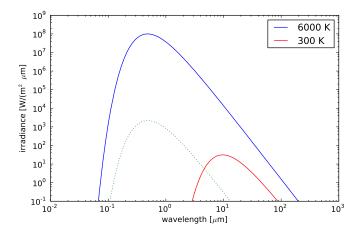


Figure: Planck functions for surface temperature of sun (\approx 6000 K, blue line), surface temperature of earth (\approx 300 K) and solar irradiance at top of atmosphere (dotted green line).

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Radiative transfer equation

$$ec{n}
abla I_{
u} = -k_{\mathrm{ext},
u} I_{
u} + rac{k_{\mathrm{sca},
u}}{4\pi} \int_{4\pi} P_{
u}(ec{n}'
ightarrow ec{n}) I_{
u}(ec{n}') d\omega + k_{\mathrm{abs},
u} B_{
u}$$

(integro-differential equation for radiance for specific direction \vec{n})

RTE includes the following processes:

- Exchange of photons with surrounding of volume element $\Delta V \Delta \omega \Delta \nu$
- Extinction
 - Absorption
 - Outscattering: Scattering of photons from \vec{n} into $\vec{n'}$
- Inscattering: Scattering of photons from $\vec{n'}$ into \vec{n}
- Emission of photons into \vec{n}

Stationary form of RTE because time dependence can be neglected in Earth's atmosphere

Single scattering properties

Molecular absorption

Direct-diffuse splitting of radiation field

total solar radiation field = diffuse solar radiation + direct solar beam

$$I_{\nu} = I_{d,\nu} + S_{\nu}\delta(\vec{n} - \vec{n_0})$$

Direct radiation S_{ν} can be separated and calculated using Lambert-Beer's law:

$$rac{\mathrm{d}S_{
u}}{\mathrm{d}s} = -k_{\mathrm{ext},
u}S_{
u}, \qquad \vec{n} = \vec{n_0}$$

RTE for diffuse solar radiation must be further simplified

Radiation	Radiative transfer equation	Discrete ordinate method	Single scattering properties	Molecular absorptic
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Horizontally homogeneous atmosphere

- plane-parallel approximation:
 - curvature of Earth's atmosphere is neglected
 - all optical properties are independent of horizontal position
 - solar beam independent on horizontal position
 - only one spatial coordinate required, altitude z or optical thickness $\tau = \int_0^z k_{\text{ext}}(z') dz'$
- approximation not valid for e.g. inhomogeneous clouds or very low sun



Figure from Mayer 2009

Discrete ordinate method

Single scattering properties

Molecular absorption

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Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Separation of μ and ϕ

- Assumption: Phase function is rotationally symmetric along direction of incident light, correct for spherical and randomly oriented particles
- Phase function expansion in Legendre series

$$\begin{split} P(\cos\Theta) &= \sum_{l=0}^{\infty} p_l P_l(\cos\Theta) \\ p_0 &= \frac{1}{2} \int_{-1}^{1} P(\cos\Theta) \mathrm{d} \cos\Theta = 1 \qquad (\textit{normalization of } P) \\ p_1 &= \frac{3}{2} \int_{-1}^{1} \cos\Theta P(\cos\Theta) \mathrm{d} \cos\Theta = g \qquad (\textit{asymmetry parameter}) \end{split}$$

 Phase function with μ = cos θ and φ separated using addition theorem of associated Legendre polynomials:

$$P(\cos \Theta) = \sum_{m=0}^{\infty} (2 - \delta_{0m}) \sum_{l=m}^{\infty} p_l^m P_l^m(\mu) P_l^m(\mu') \cos m(\phi - \phi')$$

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

System of differential equations for each Fourier mode of radiance field

• Fourier expansion of the radiance field:

$$I(au,\mu,\phi)=\sum_{m=0}^{\infty}(2-\delta_{0m})I^m(au,\mu)\cos\phi$$

 DE for each Fourier mode of radiance field, depends only on 2 variables τ and μ:

$$\mu \frac{\mathrm{d}}{\mathrm{d}\tau} I^m(\tau,\mu) = I^m(\tau,\mu) - J^m(\tau,\mu) \qquad m = 0, 1, ..., \Lambda$$

Radiation

Radiation Radiative transfer equation Discrete ordinate method

Single scattering properties

Molecular absorption

Scattering integral – Gaussian guadrature

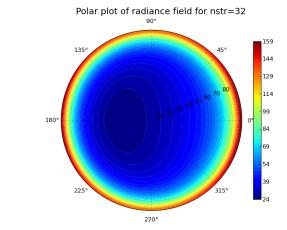
- Gaussian quadrature: method to approximate integral of functions which can well be approximated by a polynomial function
- Separate differential equation (DE) for each guadrature point (also called stream):

$$\mu_{i} \frac{\mathrm{d}I^{m}(\tau,\mu_{i})}{\mathrm{d}\tau} = I^{m}(\tau,\mu) - \frac{\omega_{0}}{2} \sum_{j=1}^{r} w_{j}I^{m}(\tau,\mu_{j}) \sum_{l=m}^{\infty} p_{l}^{m} P_{l}^{m}(\mu_{i}) P_{l}^{m}(\mu_{j})$$
$$- \frac{\omega_{0}}{4\pi} S_{0} \exp\left(-\frac{\tau}{\mu_{0}}\right) \mathcal{P}(\mu_{i},\mu_{0}) - (1-\omega_{0})B(\tau)\delta_{0m}$$

 Inhomogeneous DE ⇒ solution= particular solution for inhomogeneous DE + general solution for homogeneous DE

Molecular absorption

DOM - Impact of number of streams



- clearsky radiance field
- no aerosol ⇒ only Rayleigh scattering

Molecular absorption

DOM - Impact of number of streams

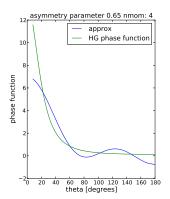
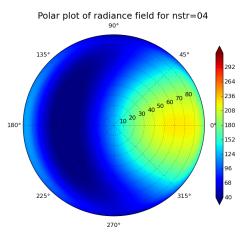


Figure: Legendre decomposition of Heney Greenstein phase function (exercise 5).



Molecular absorption

DOM - Impact of number of streams

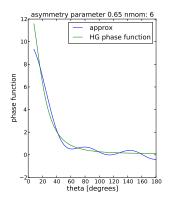
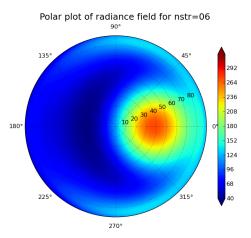


Figure: Legendre decomposition of Heney Greenstein phase function (exercise 5).



Molecular absorption

DOM - Impact of number of streams

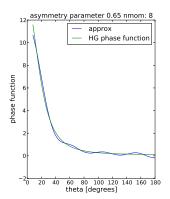
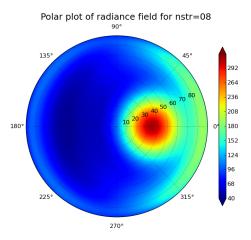


Figure: Legendre decomposition of Heney Greenstein phase function (exercise 5).



Molecular absorption

DOM - Impact of number of streams

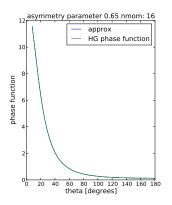
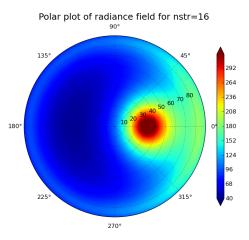


Figure: Legendre decomposition of Heney Greenstein phase function (exercise 5).



 Radiation
 Radiative transfer equation
 Discrete ordinate method
 Single scattering properties

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Molecular absorption

DOM - Impact of number of streams

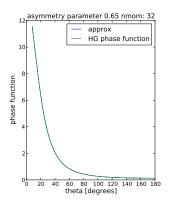
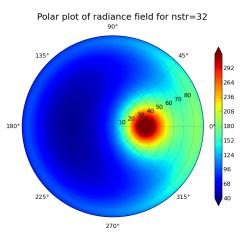


Figure: Legendre decomposition of Heney Greenstein phase function (exercise 5).



Molecular absorption

Calculation for water cloud - no deltascaling

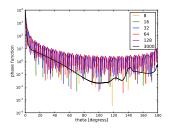


Figure: Legendre decomposition of Mie phase function (exercise 7).

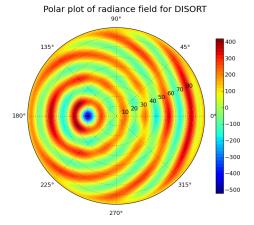


Figure: Cloudy radiance field, TOA, DISORT, nstr=16 without delta-scaling (exercise 8).

Radiation 000000	Radiative transfer equation	Discrete ordinate method	Single scattering properties	Molecular absorption

Calculation for water cloud - deltascaling on

 $P(\cos\Theta) pprox$ $2f\delta(1-\cos\Theta) + \sum_{l=0}^{2s-1} (2l+1)p_l'P_l(\cos\Theta)$

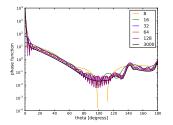


Figure: Legendre decomposition of delta-scaled Mie phase function (exercise 7).

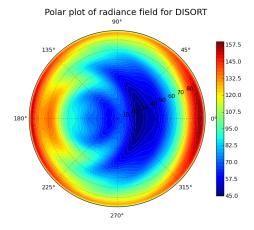


Figure: Cloudy radiance field, TOA. DISORT, nstr=16 with delta-scaling (exercise 8).

Radiative transfer equation Radiation Discrete ordinate method

Single scattering properties

Polar plot of radiance field for DISORT

Molecular absorption

157.5

145.0

132.5

120.0

107 5

95.0

82.5

70.0

575

45.0

09

45°

315°

Calculation for water cloud - intensity correction

909 135° 180° 225°

270°

Figure: Cloudy radiance field, TOA. DISORT2, nstr=16 with intensity correction (exercise 8).

DISORT2 includes intensity correction method by Nakakjima and Tanaka (1988), which calculates the first and second orders of scattering using the correct phase function

Discrete ordinate method

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Molecular absorption

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Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Single scattering theory

- Scattering calculations in planetary atmospheres:
 - single scattering by small volume element (Mie theory, geometrical optics ...)
 - 2 multiple scattering by entire atmosphere (solution of RTE, e.g. DOM)
- Assumption: scattering particles are sufficiently separated so that they can be treated as independent scatterers (no interference of radiation scattered by independent particles)

Scattered radiance at distance R in far field:

$$\vec{l}^{
m sca} = k_{
m sca} \mathbf{P} rac{\mathrm{d}V}{4\pi R^2}$$

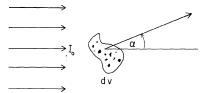


Fig. 3. Illustration of small volume element, dv, and scattering angle, $\alpha.$ Figure from Hansen and Travis, 1974

Radiation

Single scattering properties

Geometrical optics method

- Geometrical optics method can be applied for particles that are large compared to the wavelength, e.g. cloud droplets in UV/Vis
- size parameter $x = \frac{2\pi r}{\lambda} \gg 1$
- Trace individual rays through particle
- Snell's law: direction of refracted rays

 $n_1 \sin \alpha = n_2 \sin \beta$

• Fresnel equations: Intensity and polarization of radiation reflected and refracted by particle surface

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Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Geometrical optics

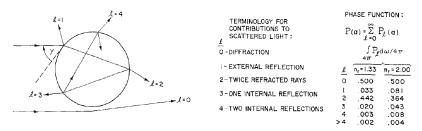


Fig. 4. Paths of light rays scattered by a sphere according to geometrical optics. $P \equiv P^{11}$ is the phase function, α the scattering angle, and y the incident angle on the sphere for rays which strike the particle. The table on the right gives the fraction of the total scattered light contained in each value of l for non-absorbing spheres with refractive indices 1.33 and 2.0.

Figure from Hansen and Travis, 1974

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Image: Image:

Molecular absorption

Rayleigh scattering

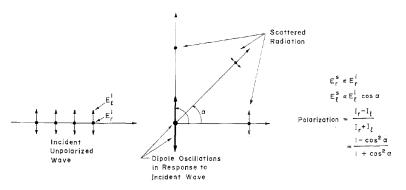


Fig. 6. Schematic representation of isotropic Rayleigh scattering. The unpolarized wave incident from the left can be represented by two linearly polarized waves vibrating at right angles to each other with equal electrical field strengths $(E_i^t = E_r^t)$ and a random phase relationship. The electrons in a small particle oscillate in response to the electric components of the incident wave, giving rise to the dipoles represented by the heavy arrow and dot. The dipole radiation is proportional to $\sin\beta$ (2.13), where $\beta = \pi/2$ for the perpendicular component and $\beta = \pi/2 - \alpha$ for the parallel component.

Figure from Hansen and Travis, 1974

Mie theory

- Calculation of optical properties (\mathbf{P} , $q_{\rm sca}$, $q_{\rm abs}$) of spherical particles (Mie, 2008)
- Solution of Maxwell equations (Input: refractive index, size parameter)
- physical explanation: multipole expansion of scattered radiation

Molecular absorption

Size distributions

 A cloud consists of droplets of various sizes following a size distribution n(r):

$$N = \int_{r_{\min}}^{r_{\max}} n(r) dr$$

optical properties are averaged over size distribution

$$\begin{aligned} k_{\rm sca} &= \int_{r_{\rm min}}^{r_{\rm max}} \sigma_{\rm sca} n(r) dr \\ k_{\rm ext} &= \int_{r_{\rm min}}^{r_{\rm max}} \sigma_{\rm ext} n(r) dr \\ \mathbf{P}(\cos \Theta) &= \frac{4\pi}{k^2 k_{\rm sca}} \int_{r_{\rm min}}^{r_{\rm max}} \mathbf{P}'(\cos \Theta, r) n(r) dr \end{aligned}$$

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Effective radius

A "mean radius" for scattering may be defined as follows (scattering cross section σ_{sca} = πr²Q_{sca}):

$$r_{\rm sca} = \frac{\int_{r_{\rm min}}^{r_{\rm max}} r \pi r^2 Q_{\rm sca}(r) n(r) dr}{\int_{r_{\rm min}}^{r_{\rm max}} \pi r^2 Q_{\rm sca}(r) n(r) dr}$$

• In the UV/VIS water cloud droplets fulfill $x\gg 1$ and $\omega_0\approx 1$, then $Q_{\rm sca}\approx 2$

$$r_{\rm eff} = \frac{1}{G} \int_{r_{\rm min}}^{r_{\rm max}} r \pi r^2 n(r) dr$$

• Generalization for non-spherical particles (e.g. ice crystals or aerosols)

$$r_{\rm eff} = \frac{\int_{r_{\rm min}}^{r_{\rm max}} V(r) n(r) dr}{\int_{r_{\rm min}}^{r_{\rm max}} A(r) n(r) dr}$$

r – equivalent sphere radius; A – geometrical cross section averaged over all possible orientations

• Effective variance of a size distribution:

$$v_{\rm eff} = \frac{1}{Gr_{\rm eff}^2} \int_{r_{\rm min}}^{r_{\rm max}} (r - r_{\rm eff})^2 A(r) n(r) dr$$

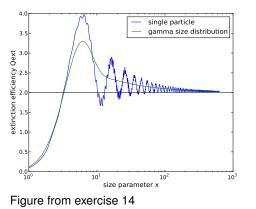
Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Extinction efficiency



- major maxima and minima
 - caused by interference of diffracted radiation (I=0) and transmitted radiation (I=2)
 - phase shift for ray passing through sphere ρ = 2x(n_r - 1)
- superimposed "ripple" structure
 - last few sigificant terms in Mie series
 - explanation: surface waves
 - vanish by integration over size distribution
- geometrical optics limit of 2 for large x

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Asymmetry parameter

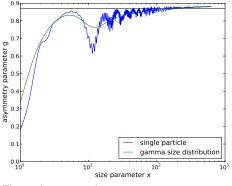


Figure from exercise 14

- geometrical optics limit of 0.87 for large x
- Rayleigh limit of 0 for small x

Radiative transfer equation

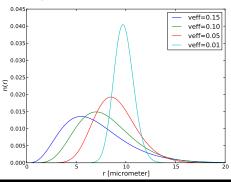
Discrete ordinate method

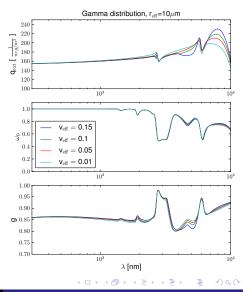
Single scattering properties

Molecular absorption

Size distributions

- Mie calculations for size distributions with the same r_{eff}=10 μm and different v_{eff} (exercise 15)
- Optical properties in UV/Vis/NIR for all size distibutions very similar, but larger differences in thermal spectral region





Radiative transfer equation

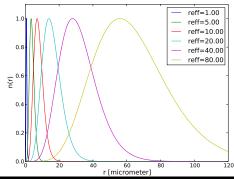
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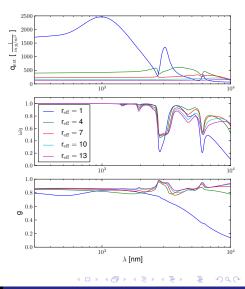
Single scattering properties

Molecular absorption

Dependence on effective radius

- Mie calculations for size distributions with different r_{eff} and the same v_{eff}=0.1 (exercise 16)
- Optical properties in UV/Vis/NIR for all size distibutions very similar, but larger differences in thermal spectral region





Radiative transfer

Radiative transfer equation

Discrete ordinate method

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Molecular absorption

Scattering phase functions

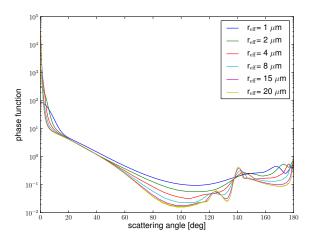
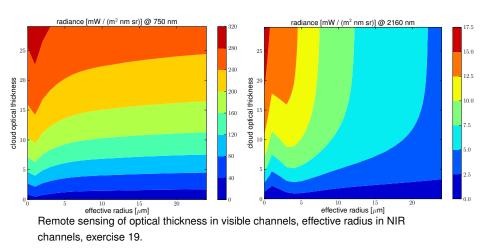


Figure: Phase functions for different effective radii at 550 nm (exercise 17).

 Radiation
 Radiative transfer equation
 Discrete ordinate method
 Single scattering properties
 Molecular absorption

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Remote sensing of clouds



Discrete ordinate method

Single scattering properties

Molecular absorption

Radiative transfer

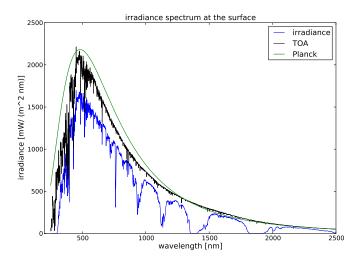
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Radiation Radiative transfer equation

Discrete ordinate method

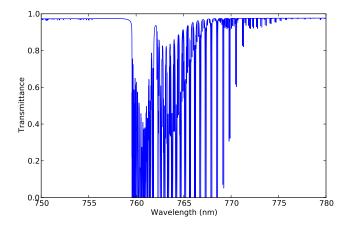
Molecular absorption •••••

Solar irradiance spectrum (surface)









libradtran calculation (line-by-line)

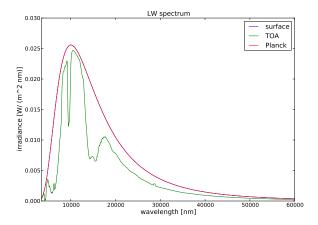
 Radiation
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Single scattering propertie

Molecular absorption

Thermal irradiance spectrum (TOA)



result from exercise 3

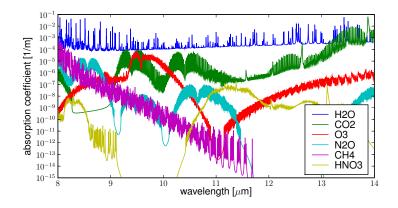
Radiative transfer equation

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Single scattering properties

Molecular absorption

Absorption coefficients in atmospheric window (8–14 μ m)



altitude: 0.5 km, ARTS calculation

Radiation

Radiation 000000	Radiative transfer equation	Discrete ordinate method	Single scattering properties	Molecular absorption

Molecular physics

Molecules have 3 forms of internal energy

$$E_{\rm int} = E_{\rm rot} + E_{\rm vib} + E_{\rm el}$$

According to quantum mechanics energy states are quantized:

- E_{rot} rotational energy (microwave)
- $E_{\rm vib}$ vibrational energy (IR)
- E_{el} electronic energy (NIR/Vis/UV)

$$E_{
m rot} < E_{
m vib} < E_{
m el}$$

- absorption: transition from lower to higher energy state
- emission: transition from higher to lower energy state
- absorption/emission lines characteristic for particular molecule

Radiation 000000	Radiative transfer equation	Discrete ordinate method	Single scattering properties	Molecular absorption
Line b	roadening			

- Natural broadening
 - Heisenberg's uncertainty priciple $\Delta E \Delta t \gtrsim h$
 - lifetime of molecule in excited state is finite
 - emitted energy is distributed over finite frequency interval $\Delta \nu$
 - negligible in Earth's atmosphere

Ollision / Pressure broadening

- during emission molecule collides with other molecules
- lifetime is shortened
- interaction causes line-broadening (larger than natural broadening because lifetime of molecule much longer than time between collisions)
- dominant below 20 km in Earth's atmosphere
- Ooppler broadening
 - random thermal motion of molecules
 - different relative velocities between molecules and radiation source causes Doppler broadening of emission lines
 - dominant above 50 km in Earth's atmosphere

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Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

Line-shapes

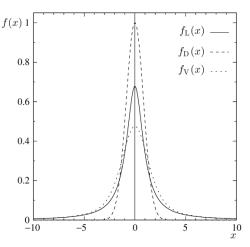


Fig. 7.5 Comparison of the Lorentz, the Doppler and the Voigt line-shape factors with $\alpha_{\rm L} = \alpha_{\rm D}$ and $x = (v - v_0)/\alpha_{\rm L}$.

Figure from Zdunkowski et al.

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

k-distribution method

- *aim:* obtain average transmission in a particular spectral band
- resort frequency grid according to absorption coefficient k and replace wavenumber integration by integration over k:

$$T_{ar{
u}} = \int_{\Delta
u} e^{-k(
u)ds} rac{d
u}{\Delta s} = \int_0^\infty e^{-kds} h(k) dk$$

- h(k) probability density function (pdf) for occurrence of k
- integration over cumulative pdf $g(k) = \int_0^k h(k) dk$:

$$T_{ar{
u}}=\int_0^1 e^{-k(g)ds}dg$$

 g(k) is a smooth monotonically increasing function between 0 and 1 and the integral can be approximated by very few grid points (e.g. using Gaussian quadrature)

Radiative transfer equation

Discrete ordinate method

Single scattering properties

Molecular absorption

k-distribution method

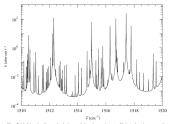


Fig. 7.10 Line-by-line calculations of the absorption coefficient for the spectral range extending from $1510-1520 \text{ cm}^{-1}$, p = 10 hPa, T = 240 K. This interval is located within the vibration–rotation water vapor band.

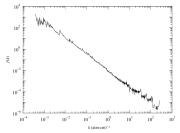


Fig. 7.11 Frequency distribution f(k) of the absorption spectrum shown in Figure 7.10.

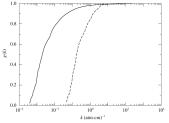


Fig. 7.12 Cumulative frequency distribution g(k) for two combinations of (p, T). Solid line: p = 10 hPa, T = 240 K, dashed line: p = 1000 hPa, T = 296 K.

Illustration of k-distribution method. Figures from Zdunkowski et al.

Discrete ordinate method

Single scattering properties

Molecular absorption

correlated-k-distribution method

- k-distribution method exact only for homogeneous layer
- for inhomogeneous atmosphere correlated-k method may be used
- Transmission for 2 trace gases:

$$(T_{ar{
u}})(1,2)=\int_{\Delta
u}T_{
u}(1)T_{
u}(2)rac{d
u}{\Delta s}$$

- Approach results in integration over two cumulative PDFs
- approximate method, accuracy investigated in e.g. Fu and Liao (1992)

Discrete ordinate method

Single scattering properties

Molecular absorption

Radiative transfer

- 1 Radiation
 - What is radiation?
 - Radiance I and irradiance E
 - Blackbody radiation
- 2 Radiative transfer equation
 - Derivation
 - Direct-diffuse splitting of radiation field
 - Horizontally homogeneous atmosphere
- Oiscrete ordinate method
 - Solution of RTE using the DOM
 - DOM Impact of number of streams
 - DOM Deltascaling and intensity correction
- 4 Single scattering properties
 - Single scattering theory
 - Size distribution
 - Examples
- Molecular absorption
 - Introduction
 - Line-by-line calculations
 - Broad-band calculations



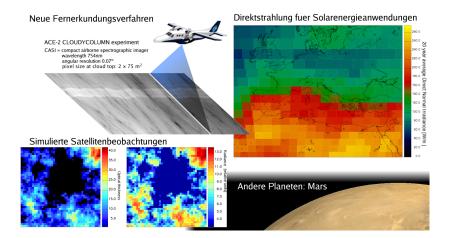
Radiative transfer equation

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Radiative transfer applications



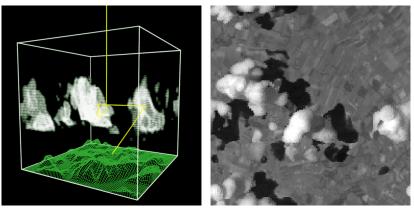
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Monte Carlo radiative transfer course



3D radiative transfer simulation using MYSTIC Monte Carlo RT course: program your own code within 1 week!