R for Photobiology

A handbook

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Preface

This is just a very early draft of a handbook that will accompany the release of the suite of R packages for photobiology (r4photobiology).

Acknowledgements

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List of abbreviations and symbols

For quantities and units used in photobiology we follow, as much as possible, the recommendations of the Commission Internationale de l'Éclairage as described by (Sliney 2007).

Symbol	**Definition**
α	absorptance (%).
Δe	water vapour pressure difference (Pa).
ϵ	emittance ($W\,m^{-2}$).
λ	wavelength (nm).
θ	solar zenith angle (degrees).
ν	frequency (Hz or s^{-1}).
ρ	reflectance (%).
σ	Stefan-Boltzmann constant.
τ	transmittance (%).
χ	water vapour content in the air ($g\,m^{-3}$).
A	absorbance (absorbance units).
ANCOVA	analysis of covariance.
ANOVA	analysis of variance.
BSWF	biological spectral weighting function.
c	speed of light in a vacuum.
CCD	charge coupled device, a type of light detector.
CDOM	coloured dissolved organic matter.
CFC	chlorofluorocarbons.
c.i.	confidence interval.
CIE	Commission Internationale de l'Éclairage; or erythemal action spectrum standardized by CIE.
CTC	closed-top chamber.
DAD	diode array detector, linear light detector based on photodiodes.
DBP	dibutylphthalate.
DC	direct current.
DIBP	diisobutylphthalate.
DNA(N)	UV action spectrum for 'naked' DNA.
DNA(P)	UV action spectrum for DNA in plants.
DOM	dissolved organic matter.
DU	Dobson units.
e	water vapour partial pressure (Pa).
E	(energy) irradiance ($W\,m^{-2}$).
$E(\lambda)$	spectral (energy) irradiance ($W\,m^{-2}\,nm^{-1}$).

E_0	fluence rate, also called scalar irradiance ($\mathrm{W\,m^{-2}}$).
ESR	early stage researcher.
FACE	free air carbon-dioxide enhancement.
FEL	a certain type of 1000 W incandescent lamp.
FLAV	UV action spectrum for accumulation of flavonoids.
FWHM	full-width half-maximum.
GAW	Global Atmosphere Watch.
GEN	generalized plant action spectrum, also abreviated as GPAS (Caldwell 1971).
GEN(G)	mathematical formulation of GEN by (Green et al. 1974) .
GEN(T)	mathematical formulation of GEN by (Thimijan et al. 1978).
h	Planck's constant.
h'	Planck's constant per mole of photons.
H	exposure, frequently called dose by biologists ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
H^{BE}	biologically effective (energy) exposure ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
$H_{\mathrm{p}}^{\mathrm{BE}}$	biologically effective photon exposure ($\mathrm{mol\,m^{-2}\,d^{-1}}$).
HPS	high pressure sodium, a type of discharge lamp.
HSD	honestly signifcant difference.
k_{B}	Boltzmann constant.
L	radiance ($\mathrm{W\,sr^{-1}\,m^{-2}}$).
LAI	leaf area index, the ratio of projected leaf area to the ground area.
LED	light emitting diode.
LME	linear mixed effects (type of statistical model).
LSD	least significant difference.
n	number of replicates (number of experimental units per treatment).
N	total number of experimental units in an experiment.
N_{A}	Avogadro constant (also called Avogadro's number).
NIST	National Institute of Standards and Technology (U.S.A.).
NLME	non-linear mixed effects (statistical model).
OTC	open-top chamber.
PAR	photosynthetically active radiation, 400–700 nm. measured as energy or photon irradiance.
PC	polycarbonate, a plastic.
PG	UV action spectrum for plant growth.
PHIN	UV action spectrum for photoinhibition of isolated chloroplasts.
PID	proportional-integral-derivative (control algorithm).
PMMA	polymethylmethacrylate.
PPFD	photosynthetic photon flux density, another name for PAR photon irradiance (Q_{PAR}).
PTFE	polytetrafluoroethylene.
PVC	polyvinylchloride.
q	energy in one photon ('energy of light').
q'	energy in one mole of photons.
Q	photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$).
$Q(\lambda)$	spectral photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}}$).
r_0	distance from sun to earth.
RAF	radiation amplification factor (nondimensional).
RH	relative humidity (%).
s	energy effectiveness (relative units).

$s(\lambda)$	spectral energy effectiveness (relative units).
s^{p}	quantum effectiveness (relative units).
$s^{\mathrm{p}}(\lambda)$	spectral quantum effectiveness (relative units).
s.d.	standard deviation.
SDK	software development kit.
s.e.	standard error of the mean.
SR	spectroradiometer.
t	time.
T	temperature.
TUV	tropospheric UV.
U	electric potential difference or voltage (e.g. sensor output in V).
UV	ultraviolet radiation (λ = 100–400 nm).
UV-A	ultraviolet-A radiation (λ = 315–400 nm).
UV-B	ultraviolet-B radiation (λ = 280–315 nm).
UV-C	ultraviolet-C radiation (λ = 100–280 nm).
$\mathrm{UV}^{\mathrm{BE}}$	biologically effective UV radiation.
UTC	coordinated universal time, replaces GMT in technical use.
VIS	radiation visible to the human eye (≈ 400–700 nm).
WMO	World Meteorological Organization.
VPD	water vapour pressure deficit (Pa).
WOUDC	World Ozone and Ultraviolet Radiation Data Centre.

Part I

Theory behind calculations

CHAPTER 1

Radiation physics

Abstract

In this chapter we explain how to .

1.1 Packages used in this chapter

For executing the examples listed in this chapter you need first to load the following packages from the library:

```
library(photobiology)

## Loading required package:  data.table

library(photobiologygg)

## Loading required package:  photobiologyWavebands
## Loading required package:  proto
## Loading required package:  ggplot2
## Loading required package:  methods
## Loading required package:  scales

library(photobiologyWavebands)
library(photobiologySun)
library(photobiologyLamps)
library(photobiologyLEDs)
```

1.2 Ultraviolet and visible radiation

Authors' note: *A much simpler, general and informal introduction to what is electromagnetic radiation is needed here before the formal description that follows.*

From the viewpoint of Physiscs, ultraviolet (UV) and visible (VIS) radiation are both considered electromagnetic waves and are described by Maxwell's equations.[1] The wavelength ranges of UV and visible radiation and their usual names are listed in Table 1.1. The long wavelengths of solar radiation, called infrared (IR) radiation, are also listed. The colour ranges indicated in Table 1.1 are an approximation as different individual human observers will not perceive colours exactly in the same way. We follow the ISO definitions for wavelength boundaries for colours (**??**). Other finer-grained colour name series are also in use (e.g. Aphalo, Albert, Björn, Ylianttila et al. 2012, Table xx)). The electromagnetic spectrum is continuous with no clear boundaries between one colour and the next, the colours could be thought as artifacts produced by our sensory system, and are meaningful only from the perspective of an *average* human observer. Especially in the IR region the subdivision is somewhat arbitrary and the boundaries used in the literature vary.

Radiation can also be thought of as composed of quantum particles or photons. The energy of a quantum of radiation in a vacuum, q, depends on the wavelength, λ, or frequency[2], ν,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \tag{1.1}$$

with the Planck constant $h = 6.626 \times 10^{-34}$ J s and speed of light in vacuum $c = 2.998 \times 10^{8}$ m s^{-1}. When dealing with numbers of photons, the equation (1.1) can be extended by using Avogadro's number $N_{\mathrm{A}} = 6.022 \times 10^{23}$ mol^{-1}. Thus, the energy of one mole of photons, q', is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \tag{1.2}$$

with $h' = h \cdot N_{\mathrm{A}} = 3.990 \times 10^{-10}$ J s mol^{-1}. Example 1: red light at 600 nm has about 200 kJ mol^{-1}, therefore, 1 µmol photons has 0.2 J. Example 2: UV-B radiation at 300 nm has about 400 kJ mol^{-1}, therefore, 1 µmol photons has 0.4 J. Equations 1.1 and 1.2 are valid for all kinds of electromagnetic waves (see Section **??** for a worked-out calculation example).

One way of understanding the relationship between the distance and positions of source and observer (or sensor) on the amount of radiation received is to use a geometric model. Bellow we describe such a model, in which a point source is located at the centre or origin of an imaginary sphere. As the distance from the origin increases, the surface area of the sphere at this distance increases. The relationship between the distance increase and area increase is, obviously, not linear. In addition, according to the well known cosine law, the amount of radiation received per unit area depends on the angle of incidence. This informal description, will is formally described below.

When a beam or the radiation passing into a space or sphere is analysed, two important parameters are necessary: the distance to the source and the

[1]These equations are a system of four partial differential equations describing classical electromagnetism.

[2]Wavelength and frequency are related to each other by the speed of light, according to $\nu = c/\lambda$ where c is speed of light in vacuum. Consequently there are two equivalent formulations for equation 1.1.

Table 1.1: Regions of the electromagnetic radiation associated with colours, after (Iqbal 1983) and (Eichler et al. 1993) with alterations.

Colour	Wavelength (nm)	Frequency (THz)
UV-C	100 – 280	3000 – 1070
UV-B	280 – 315	1070 – 950
UV-A	315 – 400	950 – 750
violet	400 – 455	750 – 660
blue	455 – 492	660 – 610
green	492 – 577	610 – 520
yellow	577 – 597	520 – 502
orange	597 – 622	502 – 482
red	622 – 700	482 – 428
far red	700 – 770	428 – 390
near IR	770 – 3000	390 – 100
mid IR	3000 – 50000	100 – 6
far IR	50000 – 10^6	6 – 0.3

measuring position—i.e. if the receiving surface is perpendicular to the beam or not. The geometry is illustrated in Figure 1.1 with a radiation source at the origin. The radiation is received at distance r by a surface of area dA, tilted by an angle α to the unit sphere's surface element, so called solid angle, dΩ, which is a two-dimensional angle in a space. The relation between dA and dΩ in spherical coordinates is geometrically explained in Figure 1.1.

The solid angle is calculated from the zenith angle θ and azimuth angle ϕ, which denote the direction of the radiation beam

$$\mathrm{d}\Omega = \mathrm{d}\theta \cdot \sin\theta \mathrm{d}\phi \tag{1.3}$$

The area of the receiving surface is calculated by a combination of the solid angle of the beam, the distance r from the radiation source and the angle α of the tilt:

$$\mathrm{d}A = \frac{r\mathrm{d}\theta}{\cos\alpha} \cdot r\sin\theta\mathrm{d}\phi \tag{1.4}$$

which can be rearranged to

$$\Rightarrow \mathrm{d}A = \frac{r^2}{\cos\alpha} \quad \mathrm{d}\Omega \tag{1.5}$$

Thus, the solid angle is given by

$$\Omega = \int_A \frac{\mathrm{d}A \cdot \cos\alpha}{r^2} \tag{1.6}$$

The unit of the solid angle is a steradian (sr). The solid angle of an entire sphere is calculated by integration of equation (1.3) over the zenith (θ) and azimuth (ϕ) angles, $0 \le \theta \le \pi(180°)$ and $0 \le \phi \le 2\pi(360°)$, and is 4π sr. For example, the sun or moon seen from the Earth's surface appear to have a diameter of about 0.5° which corresponds to a solid angle element of about 6.8×10^{-5} sr.

When radiation travels through a medium it can be absorbed (the energy 'taken up' by the material's atoms) or scattered (the direction of travel of the

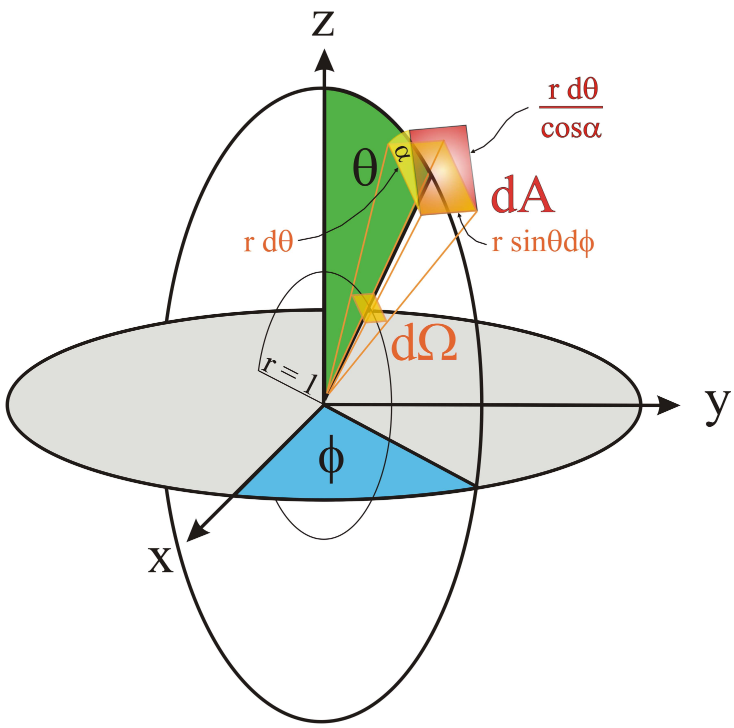


Figure 1.1: Definition of the solid angle dΩ and the geometry of areas in the space (redrawn after Eichler et al. 1993), where the given solid angle dΩ remains the same, regardless of distance r, while the exposed area exemplified by dA will change with distance r from the origin (light source) and the angle α, if the exposed area (or detector) is tilted. The angle denoted by ϕ is the azimuth angle and θ is the zenith angle.

radiation randomly altered). Both of these phenomena affect the amount of radiation that reaches the 'other end of the path' where the observer or sensor is located, and their effect depends on the length of the path. Once again, this informal description, is stated formally below.

The processes responsible for the variation of the radiance $L(\lambda, \theta, \phi)$ as the radiation beam travels through any kind of material, are primarily absorption a and scattering b, which are called inherent optical properties, because they depend only on the characteristics of the material itself and are independent of the light field. Radiance is added to the directly transmitted beam, coming from different directions, due to elastic scattering, by which a photon changes direction but not wavelength or energy level. An example of this is Raleigh scattering in very small particles, which causes the scattering of light in a rainbow. A further gain of radiance into the direct path is due to inelastic processes like fluorescence, where a photon is absorbed by the material and reemitted as a photon with a longer wavelength and lower energy level, and Raman scattering. The elastic and inelastic scattered radiance is denoted as L^E and L^I, respectively. Internal sources of radiances, L^S, like bioluminescence of biological organisms or cells contribute also to the detected radiance. The path of the radiance through a thin horizontal layer with thickness d$z = z_1 - z_0$ is shown schematically in Figure 1.2.

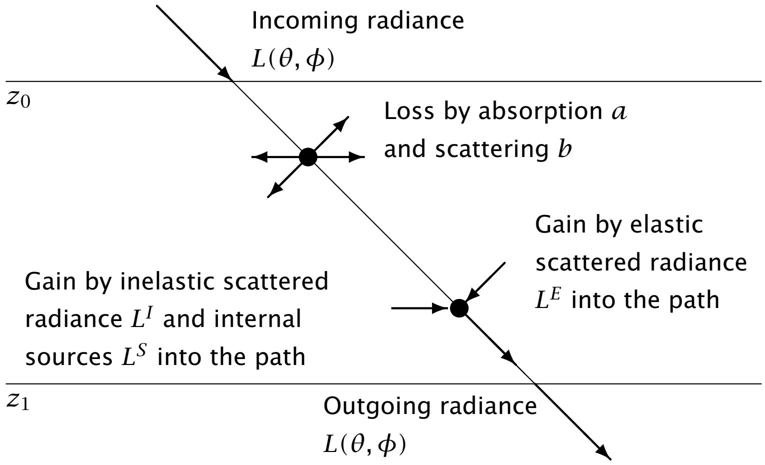


Figure 1.2: Path of the radiance and influences of absorbing and scattering particles in a thin homogeneous horizontal layer of air or water. The layer is separated from other layers of different characteristics by boundary lines at height z_0 and z_1.

Putting all this together, the radiative transfer equation is

$$\cos\theta \, \frac{\mathrm{d}L}{\mathrm{d}z} = -(a+b) \cdot L + L^E + L^I + L^S \tag{1.7}$$

The dependencies of L on λ, θ, and ϕ are omitted here for brevity. No exact analytical solution to the radiative transfer equation exists, hence it is necessary either to use numerical models or to make approximations and find an analytical parameterisation. A numerical model is for example the Monte Carlo method. The parameters of the light field can be simulated by modelling the paths of photons. For an infinite number of photons the light field parameters reach their exact values asymptotically. The advantage of the Monte Carlo method is a relatively simple structure of the program, and it simulates nature in a straightforward way, but its disadvantage is the time-consuming computation involved. Details of the Monte Carlo method are explained for example by (Prahl et al. 1989), (Wang et al. 1995)[3], or (Mobley 1994).

The other way to solve the radiative transfer equation is through the development of analytical parameterisations by making approximations for all the quantities needed. In this case, the result is not exact, but it has the advantage of fast computing and the analytical equations can be inverted just as fast. This leads to the idealised case of a source-free ($L^S = 0$) and non-scattering media, i.e. $b = 0$ and therefore $L^E = L^I = 0$. Then, equation 1.7 can be integrated easily and yields

$$L(z_1) = L(z_0) \cdot \mathrm{e}^{-\frac{a \cdot (z_1 - z_0)}{\cos\theta}} \tag{1.8}$$

[3]Their program is available from the website of Oregon Medical Laser Center at http://omlc.ogi.edu/software/mc/

The boundary value $L(z_0)$ is presumed known. This result is known as Beer's law (or Lambert's law, Bouguer's law, Beer-Lambert law), denotes any instance of exponential attenuation of light and is exact only for purely absorbing media—i.e. media that do not scatter radiation. It is of direct application in analytical chemistry, as it describes the direct proportionality of absorbance (A) to the concentration of a coloured solute in a transparent solvent.

Table 1.2: Physical quantities of light.

Symbol	Unit	Description
$\Phi = \frac{\partial q}{\partial t}$	W = J s^{-1}	Radiant flux: absorbed or emitted energy per time interval
$H = \frac{\partial q}{\partial A}$	J m^{-2}	Exposure: energy towards a surface area. (In plant research this is called usually *dose* (H), while in Physics *dose* refers to absorbed radiation.)
$E = \frac{\partial \Phi}{\partial A}$	W m^{-2}	Irradiance: flux or radiation towards a surface area, radiant flux density
$I = \frac{\partial \Phi}{\partial \Omega}$	W sr^{-1}	Radiant intensity: emitted radiant flux of a surface area per solid angle
$\epsilon = \frac{\partial \Phi}{\partial A}$	W m^{-2}	Emittance: emitted radiant flux per surface area
$L = \frac{\partial^2 \Phi}{\partial \Omega (\partial A \cdot \cos \alpha)} = \frac{\partial I}{\partial A \cdot \cos \alpha}$	W m^{-2} sr^{-1}	Radiance: emitted radiant flux per solid angle and surface area depending on the angle between radiant flux and surface perpendicular

Different physical quantities are used to describe the "amount of radiation" and their definitions and abbreviations are listed in Table 1.2. Taking into account Equation 1.6 and assuming a homogenous flux, the important correlation between irradiance E and intensity I is

$$E = \frac{I \cdot \cos \alpha}{r^2} \tag{1.9}$$

The irradiance decreases by the square of the distance to the source and depends on the tilt of the detecting surface area. This is valid only for point sources. For outdoor measurements the sun can be assumed to be a point source. For artificial light sources simple LEDs (light-emitting diodes) without optics on top are also effectively point sources. However, LEDs with optics—and other artificial light sources with optics or reflectors designed to give a more focused dispersal of the light—deviate to various extents from the rule of a decrease of irradiance proportional to the square of the distance from the light source.

Besides the physical quantities used for all electromagnetic radiation, there are also equivalent quantities to describe visible radiation, so called photometric quantities. The human eye as a detector led to these photometric units, and they are commonly used by lamp manufacturers to describe their artificial light sources. See Box **??** on page **??** for a short description of these quantities and units.

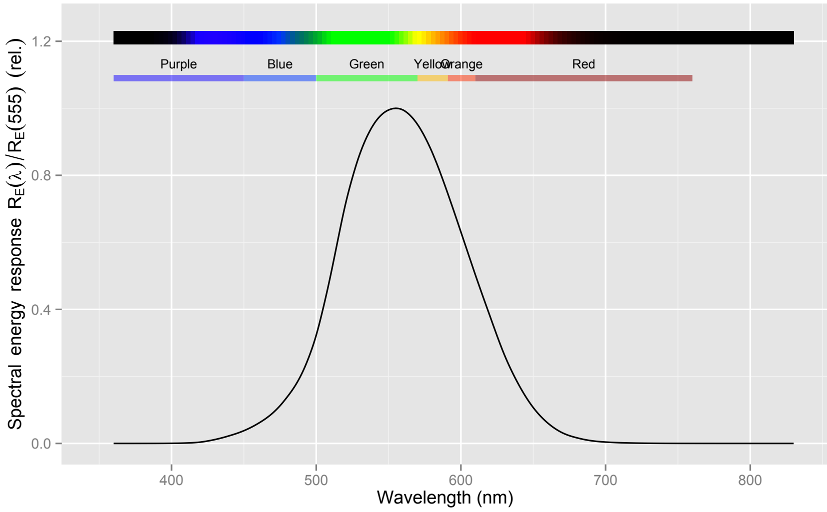
Photometric quantities

In contrast to (spectro-)radiometry, where the energy of any electromagnetic radiation is measured in terms of absolute power ($\mathrm{J\,s} = W$), photometry measures light as perceived by the human eye. Therefore, radiation is weighted by a luminosity function or visual sensitivity function describing the wavelength dependent response of the human eye. Due to the physiology of the eye, having rods and cones as light receptors, different sensitivity functions exist for the day (photopic vision) and night (scotopic vision), $V(\lambda)$ and $V'(\lambda)$, respectively. The maximum response during the day is at $\lambda = 555$ nm and during night at $\lambda = 507$ nm. Both response functions (normalised to their maximum) are shown in the figure below as established by the Commission Internationale de l'Éclairage (CIE, International Commission on Illumination, Vienna, Austria) in 1924 for photopic vision and 1951 for scotopic vision (Schwiegerling 2004). The data are available from the Colour and Vision Research Laboratory at `http://www.cvrl.org`. Until now, $V(\lambda)$ is the basis of all photometric measurements.

Corresponding to the physical quantities of radiation summarized in the table 1.2, the equivalent photometric quantities are listed in the table below and have the subscript v. The ratio between the (physiological) luminous flux Φ_v and the (physical) radiant flux Φ is the (photopic) photometric equivalent $K(\lambda) = V(\lambda) \cdot K_m$ with $K_m = 683$ lm W^{-1} (lumen per watt) at 555 nm. The dark-adapted sensitivity of the eye (scotopic vision) has its maximum at 507 nm with 1700 lm W^{-1}. The base unit of luminous intensity is candela (cd). One candela is defined as the monochromatic intensity at 555 nm (540 THz) with $I = \frac{1}{683}$ W sr^{-1}. The luminous flux of a normal candle is around 12 lm. Assuming a homogeneous emission into all directions, the luminous intensity is about $I_\mathrm{v} = \frac{12\ \mathrm{lm}}{4\pi\ \mathrm{sr}} \approx 1$ cd.

Photon or quantum quantities of radiation.

When we are interested in photochemical reactions, the most relevant radiation quantities are those expressed in photons. The reason for this is that, as discussed in section **??** on page **??**, molecules are excited by the absorption of certain fixed amounts of energy or quanta. The surplus energy “decays” by non-photochemical processes. When studying photosynthesis, where many photons of different wavelengths are simultaneously important, we normally use photon irradiance to describe amount of PAR. The name photosynthetic



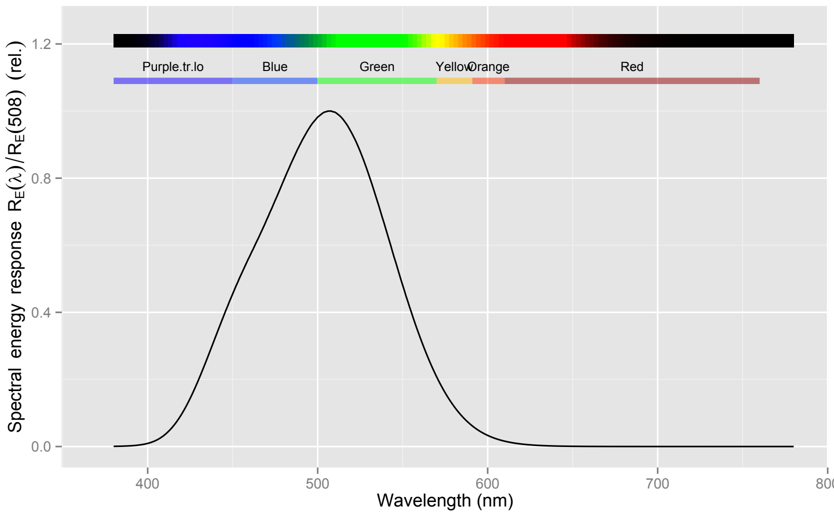


Figure 1.3: Relative spectral intensity of human colour sensation during day (solid line) and night (dashed line), $V(\lambda)$ and $V'(\lambda)$ respectively.

photon flux density, or PPFD, is also frequently used when referring to PAR photon irradiance. When dealing with energy balance of an object instead of photochemistry, we use (energy) irradiance. In meteorology both UV and visible radiation, are quantified using energy-based quantities. When dealing with UV photochemistry as in responses mediated by UVR8, an UV-B photoreceptor, the use of quantum quantities is preferred. According to the physical energetic quantities in the table 1.2, the equivalent photon related quantities are listed in the table below and have the subscript p.

These quantities can be also used based on a 'chemical' amount of moles by dividing the quantities by Avogadro's number $N_A = 6.022 \times 10^{23}$ mol^{-1}. To determine a quantity in terms of photons, an energetic quantity has to

Table 1.3: Photometric quantities of light.

Symbol	Unit	Description
q_v	lm s	Luminous energy or quantity of light
$\Phi_\mathrm{v} = \frac{\partial q_\mathrm{v}}{\partial t}$	lm	Luminous flux: absorbed or emitted luminous energy per time interval
$I_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial \Omega}$	cd = lm sr^{-1}	Luminous intensity: emitted luminous flux of a surface area per solid angle
$E_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial A}$	lux = lm m^{-2}	Illuminance: luminous flux towards a surface area
$\epsilon_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial A}$	lux	Luminous emittance: luminous flux per surface area
$H_\mathrm{v} = \frac{\partial q_\mathrm{v}}{\partial A}$	lux s	Light exposure: quantity of light towards a surface area
$L_\mathrm{v} = \frac{\partial^2 \Phi_\mathrm{v}}{\partial \Omega (\partial A \cdot \cos\alpha)} = \frac{\partial I_\mathrm{v}}{\partial A \cdot \cos\alpha}$	cd m^{-2}	Luminance: luminous flux per solid angle and surface area depending on the angle between luminous flux and surface perpendicular

Table 1.4: Photon quantities of light.

Symbol	Unit	Description
Φ_p	s^{-1}	Photon flux: number of photons per time interval
$Q = \frac{\partial \Phi_\mathrm{p}}{\partial A}$	$\mathrm{m}^{-2}\ \mathrm{s}^{-1}$	Photon irradiance: photon flux towards a surface area, photon flux density (sometimes also symbolised by E_p)
$H_\mathrm{p} = \int_t Q\ \mathrm{d}t$	m^{-2}	Photon exposure: number of photons towards a surface area during a time interval, photon fluence

be weighted by the number of photons, i.e. divided by the energy of a single photon at each wavelength as defined in equation 1.1. This yields for example

$$\Phi_\mathrm{p} = \frac{\lambda}{h\ c} \cdot \frac{\partial q}{\partial t} \qquad \text{and} \qquad Q(\lambda) = \frac{\lambda}{h\ c} \cdot E(\lambda)$$

Photon or quantum quantities of radiation.

When dealing with bands of wavelengths, for example an integrated value like PAR from 400 to 700 nm, it is necessary to repeat these calculations at each wavelength and then integrate over the wavelengths. For example, the PAR photon irradiance or PPFD in moles of photons is obtained by

$$\mathrm{PPFD} = \frac{1}{N_\mathrm{A}} \int_{400\,\mathrm{nm}}^{700\,\mathrm{nm}} \frac{\lambda}{hc}\ E(\lambda)\ \mathrm{d}\lambda$$

For integrated values of UV-B or UV-A radiation the calculation is done analogously by integrating from 280 to 315 nm or 315 to 400 nm, respectively.

If we have measured (energy) irradiance, and want to convert this value to photon irradiance, the exact conversion will be possible only if we have information about the spectral composition of the measured radiation. Conversion factors at different wavelengths are given in the table below. For PAR, 1 $\mathrm{W\,m^{-2}}$ of "average daylight" is approximately 4.6 $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$. This is exact only if the radiation is equal from 400 to 700 nm, because the factor is the value at the central wavelength at 550 nm. Further details are discussed in section **??** on page **??**.

Table 1.5: Conversion factors of photon and energy quantities at different wavelengths.

	$\mathrm{W\,m^{-2}}$ to $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$	λ (nm)
	2.34	280
UV-B	2.49	298
	2.63	315
UV-A	2.99	358
	3.34	400
PAR	4.60	550
	5.85	700

There are, in principle, two possible approaches to measuring radiation. The first is to observe light from one specific direction or viewing angle, which is the radiance L. The second is to use a detector, which senses radiation from more than one direction and measures the so-called irradiance E of the entire sphere or hemisphere. The correlation between irradiance E and radiance L of the wavelength λ is given by integrating over all directions of incoming photons.

$$E_0(\lambda) = \int_\Omega L(\lambda, \Omega)\,\mathrm{d}\Omega \tag{1.10}$$

$$E(\lambda) = \int_\Omega L(\lambda, \Omega)\,|\cos\alpha|\,\mathrm{d}\Omega \tag{1.11}$$

Depending on the shape of a detector (which may be either planar or spherical) the irradiance is called (plane) irradiance E or fluence rate (also called scalar irradiance) E_0. A planar sensor detects incoming photons depending on the incident angle and a spherical sensor detects all photons equally weighted for all directions. See section **??** on page **??** for a more detailed discussion.

Here we have discussed the properties of light based on energy quantities. In photobiology there are good reasons to quantify radiation based on photons. See Box **??** on page **??**, and section **??** on page **??**.

1.3 Solar radiation

When dealing with solar radiation, we frequently need to describe the position of the sun. The azimuth angle (ϕ) is measured clockwise from the North on a horizontal plane. The position on the vertical plane is measured either as the zenith angle (θ) downwards from the zenith, or as an elevation angle (h)

upwards from the horizon. Consequently $h + \theta = 90° = \frac{\pi}{2}$ radians. See Figure 1.4 for a diagram. In contrast to Figure 1.1 and the discussion in section ?? where the point radiation source is located at the origin of the system of coordinates, when describing the position of the sun as in Figure 1.4 the observer is situated at the origin.

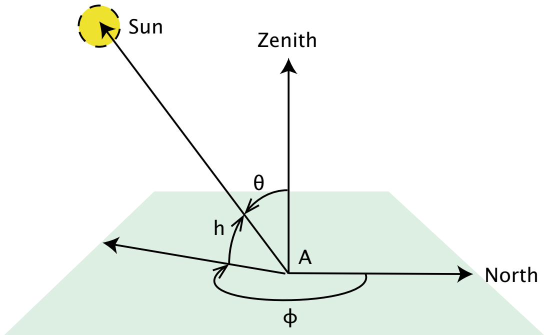


Figure 1.4: Position of the sun in the sky and the different angles used for its description by an observer located at point A. The azimuth angle is ϕ, the elevation angle is h and the zenith angle is θ. These angles are measured on two perpendicular planes, one horizontal and one vertical.

Ultraviolet and visible radiation are part of solar radiation, which reaches the Earth's surface in about eight minutes (t = time, r_0 = distance sun to earth, c = velocity of light in vacuum):

$$t = \frac{r_0}{c} \approx \frac{150 \times 10^9 \text{ m}}{3 \times 10^8 \frac{\text{m}}{\text{s}}} = 500 \text{ s} = 8.3 \text{ min}$$

The basis of all passive measurements is the incoming solar radiation, which can be estimated from the known activity of the sun ('productivity of photons'), that can be approximated by the emitted spectral radiance (L_s) described by Planck's law of black body radiation at temperature T, measured in degrees Kelvin (K):

$$L_\text{s}(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{\mathrm{e}^{(hc/k_\text{B}T\lambda)} - 1} \tag{1.12}$$

with Boltzmann's constant $k_\text{B} = 1.381 \times 10^{-23}\ \text{JK}^{-1}$. The brightness temperature of the sun can be determined by Wien's displacement law, which gives the peak wavelength of the radiation emitted by a blackbody as a function of its absolute temperature

$$\lambda_{max} \cdot T = 2.898 \times 10^6 \,\text{nm}\,\text{K} \tag{1.13}$$

This means that for a maximum emission of the sun at about 500 nm the temperature of the sun surface is about 5800 K. The spectral irradiance of the sun $E_\text{s}(\lambda)$ can be estimated assuming a homogeneous flux and using the correlation of intensity I and radiance L from their definitions in table 1.2. The intensity of the sun $I_\text{s}(\lambda)$ is given by the radiance $L_\text{s}(\lambda)$ multiplied by the apparent sun surface (a non-tilted disk of radius $r_s = 7 \times 10^5$ km). To calculate the decreased solar irradiance at the moment of reaching the Earth's atmosphere, the distance of the sun to the Earth ($r_0 = 150 \times 10^6$ km) has to be taken into account due to the inverse square law of irradiance of equation (1.9). Thus, the extraterrestrial solar irradiance is

$$E_{\mathrm{s}}(\lambda) = L_{\mathrm{s}}(\lambda) \cdot \frac{\pi r_s^2}{r_0^2} \tag{1.14}$$

Remembering the solid angle of equation (1.6), the right multiplication factor represents the solid angle of the sun's disk as seen from the Earth's surface ($\approx 6.8 \times 10^{-5}$ sr). Figure 1.5 shows the spectrum of the measured extraterrestrial solar radiation (Wehrli, 1985)[4] and the spectrum calculated by equation 1.14 using Planck's law of equation 1.12 at a black body temperature of 5800 K. Integrated over all wavelengths, E_{s} is about 1361 to 1362 $\mathrm{W\,m^{-2}}$ at top of the atmosphere (Kopp and Lean 2011). This value is called the 'solar constant'. In former times, depending on different measurements, E_{s} varies by a few percent (Iqbal 1983). For example, the irradiance at the top of the atmosphere (the integrated value) changes by ± 50 $\mathrm{W\,m^{-2}}$ (3.7 %) during the year due to distance variation caused by orbit excentricity (Mobley 1994). More accurate measurements during the last 25 years by spaceborne radiometers show a variability of the solar radiation of a few tenth of a percent. A detailed analysis is given by (Fröhlich and Lean 2004). E_{s} can also be calculated by the Stefan-Boltzmann Law: the total energy emitted from the surface of a black body is proportional to the fourth power of its temperature. For an isotropically emitting source (Lambertian emitter), this means

$$L = \frac{\sigma}{\pi} \cdot T^4 \tag{1.15}$$

with the Stefan-Boltzmann constant $\sigma = 5.6705 \times 10^{-8}$ W m^{-2} K^{-4}. With $T = 5800$ K equation 1.15 gives the radiance of the solar disc. From this value, we can obtain an approximation of the solar constant, by taking into account the distance from the Earth to the Sun and the apparent size of the solar disc (see equations 1.6 and 1.9).

The total solar irradiance covers a wide range of wavelengths. Using some of the 'colours' introduced in table 1.1, table 1.6 lists the irradiance and fraction of E_{s} of different wavelength intervals.

The extraterrestrial solar spectrum differs from that at ground level due to the absorption of radiation by the atmosphere, because the absorption peaks of water, CO_2 and other components of the atmosphere, cause corresponding valleys to appear in the solar spectrum at ground level. For example, estimates from measurements of the total global irradiance at Helmholtz Zentrum München (11.60° E, 48.22° N, 490 m above sea level) on two sunny days (17$^{\mathrm{th}}$ April 1996, sun zenith angle of 38° and 27$^{\mathrm{th}}$ May 2005, 27°) result in about 5% for wavelengths below 400 nm, about 45% from 400 to 700 nm, and about 50% above 700 nm. In relation to plant research, only the coarse structure of peaks and valleys is relevant, because absorption spectra of pigments *in vivo* have broad peaks and valleys. However, the solar spectrum has a much

[4]Available as ASCII file at PMODWRC, ftp://ftp.pmodwrc.ch/pub/publications/pmod615.asc

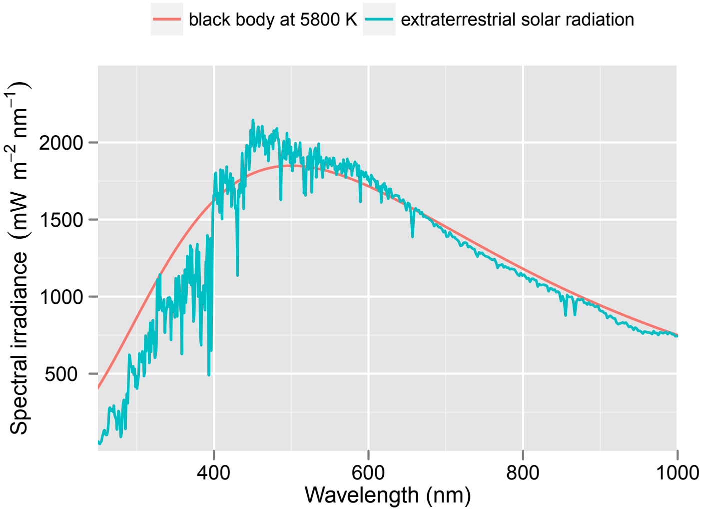


Figure 1.5: Extraterrestrial solar spectrum after (Wehrli 1985) (green line) and spectrum of a black body at 5800 K (red line), calculated using Planck's law (equation 1.12) and converted to extraterrestrial spectral irradiance with equation 1.14.

Table 1.6: Distribution of the extraterrestrial solar irradiance E_s constant in different wavelength intervals calculated using the data of (Wehrli 1985) shown in Figure 1.5.

Colour	Wavelength (nm)	Irradiance ($W m^{-2}$)	Fraction of E_s (%)
UV-C	100 – 280	7	0.5
UV-B	280 – 315	17	1.2
UV-A	315 – 400	84	6.1
VIS	400 – 700	531	38.9
near IR	700 – 1 000	309	22.6
mid and far IR	> 1 000	419	30.7
total		1 367	100.0

Figure 1.6: Sky photos in different portions of the light spectrum. They show that in the UV-A band the diffuse component is proportionally larger than it is at longer wavelengths. This can be seen as reduced contrast. Photographs taken by L. Ylianttila at the fortress of Suomenlinna (`http://www.suomenlinna.fi/en`), Helsinki, Finland.

finer structure, due to emission and absorption lines of elements, which is not observable with the spectroradiometers normally used in plant research.

At the Earth's surface, the incident radiation or *global radiation* has two components, direct radiation and scattered or 'diffuse' radiation. Direct radiation is radiation travelling directly from the sun, while diffuse radiation is that scattered by the atmosphere. Diffuse radiation is what gives the blue colour to the sky and white colour to clouds. The relative contribution of direct and diffuse radiation to global radiation varies with wavelength and weather conditions. The contribution of diffuse radiation is larger in the UV region, and in the presence of clouds (Figures 1.6 and 1.7).

Not only total irradiance, but also the wavelength distribution of the solar spectrum changes with the seasons of the year and time of day. The spectral wavelength distribution is also changed by the amount of UV-absorbing ozone in the atmosphere, known as the ozone column. Figure 1.8 shows how spectral irradiance changes throughout one day. When the whole spectrum is plotted using a linear scale the effect of ozone depletion is not visible, however, if we plot only the UV region (Figure 1.9) or use a logarithmic scale (Figure 1.10), the effect becomes clearly visible. In addition, on a log scale, it is clear that the relative effect of ozone depletion on the spectral irradiance at a given wavelength increases with decreasing wavelength.

Seasonal variation in UV-B irradiance has a larger relative amplitude than variation in PAR (Figure 1.11). This causes a seasonal variation in the UV-B: PAR ratio (Figure 1.12). In addition to the regular seasonal variation, there is random variation as a result of changes in clouds (Figure 1.12). Normal seasonal and spatial variation in UV can be sensed by plants, and could play a role in their adaptation to seasons and/or their position in the canopy.

UV-B irradiance increases with elevation in mountains and with decreasing latitude (Figure 1.13) and is particularly high on high mountains in equatorial regions. This has been hypothesized to be a factor in the determination of the tree line[5] in these mountains (Flenley 1992).

An increase in the UV-B irradiance is caused by depletion of the ozone layer in the stratosphere, mainly as a consequence of the release of chlorofluorocarbons (CFCs), used in cooling devices such as refrigerators and air conditioners, and in some spray cans (see Graedel and Crutzen 1993). The most dramatic manifestation of this has been the seasonal formation of an "ozone hole" over Antarctica. It is controversial whether a true ozone hole has already formed in the Arctic, but strong depletion has occurred in year 2011 (Manney et al. 2011) and atmospheric conditions needed for the formation of a "deep" ozone hole are not very different from those prevalent in recent years. Not so

[5] *Tree line* is the highest elevation on a mountain slope at which tree species are naturally able to grow.

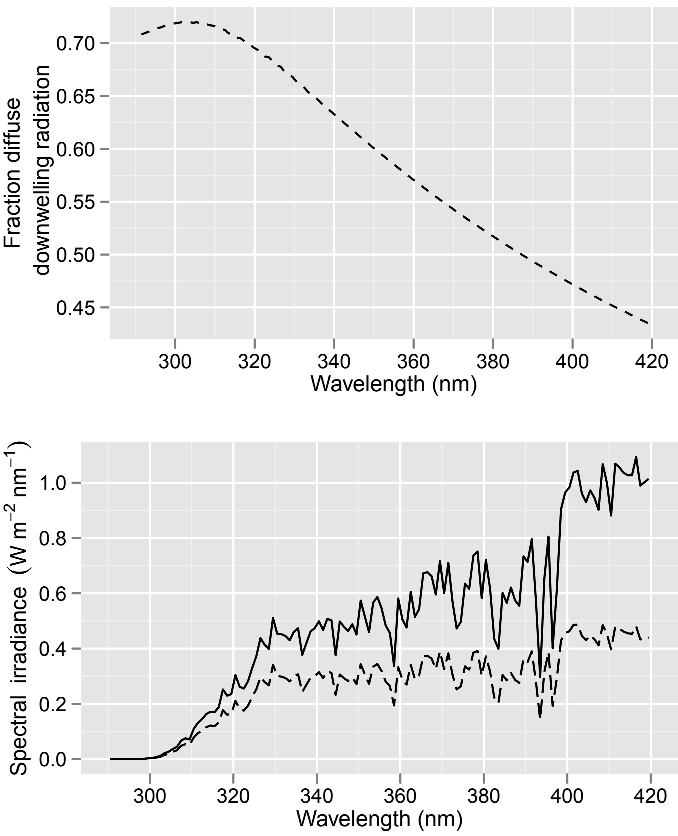


Figure 1.7: Diffuse component in solar UV. Spectral irradiance of total downwelling radiation (lower panel, solid line), diffuse downwelling radiation (lower panel, long dashes), and ratio of diffuse downwelling to total downwelling spectral irradiance (upper panel, dashed line) are shown. Data from TUV model (version 4.1) for solar zenith angle = $40°00'$, cloud-free conditions, 300 Dobson units. Simulations done with the Quick TUV calculator at `http://cprm.acd.ucar.edu/Models/TUV/Interactive_TUV/`.

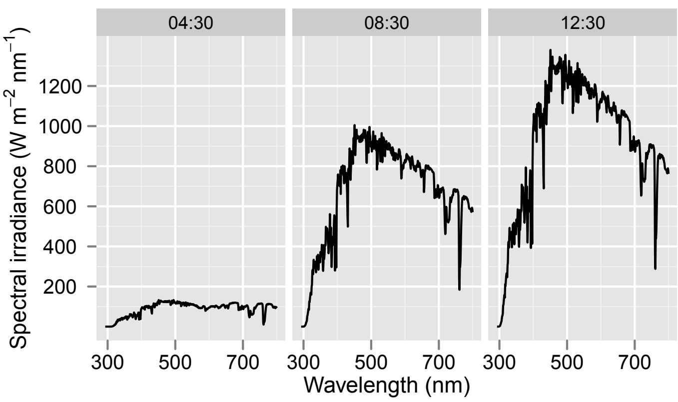


Figure 1.8: The solar spectrum through half a day. Simulations of global radiation (direct plus diffuse radiation) spectral irradiance on a horizontal surface at ground level) for a hypothetical 21 May with cloudless sky at Jokioinen (60°49'N, 23°30'E), under normal ozone column conditions. Effect of depletion is so small on the solar spectrum as a whole, that it would not visible in this figure. See (Kotilainen et al. 2011) for details about the simulations.

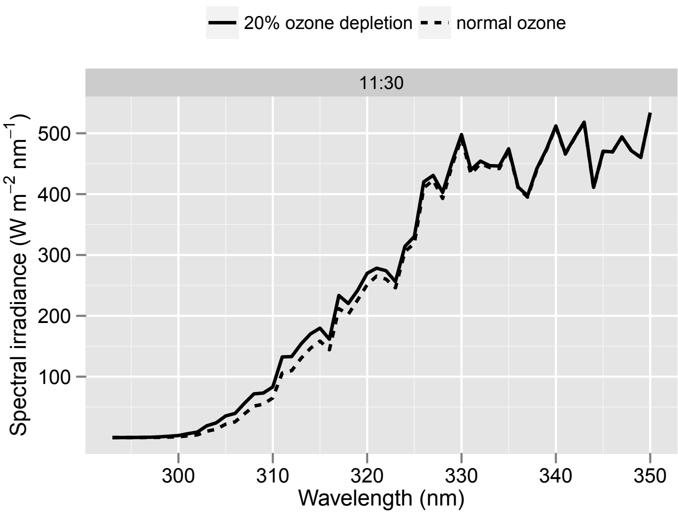


Figure 1.9: The effect of ozone depletion on the UV spectrum of global (direct plus diffuse) solar radiation at noon. See fig. 1.8 for details.

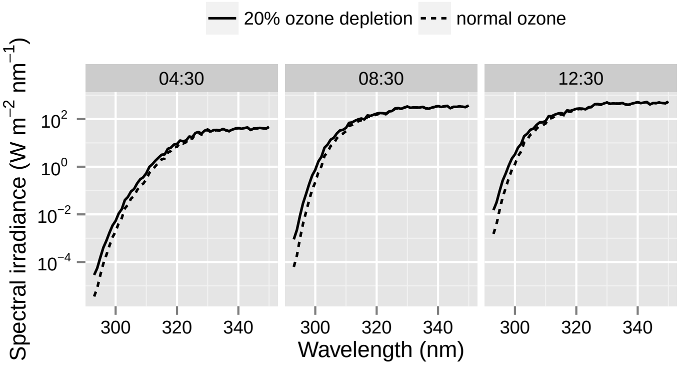


Figure 1.10: The solar UV spectrum through half a day. The effect of ozone depletion on global (direct plus diffuse) radiation. A logarithmic scale is used for spectral irradiance. See fig. 1.8 for details.

Figure 1.11: UV-B and PAR. Left: Diffuse radiation as percentage of total (direct + diffuse) radiation in the UV-B (solid line) and PAR (dashed line) wavebands for open areas in a humid temperate climate under a clear sky. In cloudy conditions the percentage of diffuse radiation increases. Day of year not specified. Redrawn from (Flint and Caldwell 1998). Right: Seasonal variation in modelled, clear sky, solar-noon, UV-B (solid line) and PAR (dashed line) irradiance above the canopy for Maryland, USA. Irradiance expressed relative to annual maximum of each waveband. Adapted from (Brown et al. 1994).

Figure 1.12: Seasonal variation in UV-B radiation at Erlangen, Germany (54° 10’ N, 07° 51’ E, 280 m asl). (Top) UV-B:PAR energy ratio, calculated from daily exposures, and (bottom) UV-B daily exposure, measured with ELDONET instruments (see Figure 2 in Häder et al. 2007, for details).

dramatic, but consistent, depletion has also been observed at mid-latitudes in both hemispheres. CFCs and some other halocarbons have been phased out following the Montreal agreement and later updates. However, as CFCs have a long half life in the atmosphere, of the order of 100 years, their effect on the ozone layer will persist for many years, even after their use has been drastically reduced. Model-based predictions of changes in atmospheric circulation due to global climate change have been used to derive future trends in UV index and ozone column thickness (Hegglin and Shepherd 2009). In addition, increased cloudiness and pollution, could lead to decreased UV and PAR, sometimes called ‘global dimming’ (e.g. Stanhill and Cohen 2001). It should be noted that, through reflection, broken clouds can locally increase UV irradiance to values above those under clear-sky conditions (S. B. Díaz et al. 1996; Frederick et al. 1993).

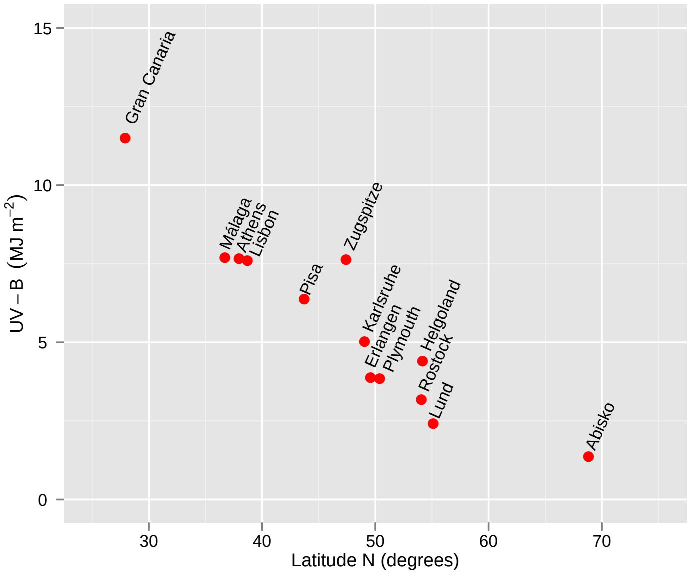


Figure 1.13: Latitudinal variation in UV-B radiation in the Northern hemisphere. UV-B annual exposure, measured with ELDONET instruments (see Häder et al. 2007, for details).

1.4 Artificial radiation

Different types of man-made VIS and UV radiation sources exist, based on exploiting different physical phenomena.

Incandescent light sources are “black bodies” heated at a very high temperature. Normal incandescent lamps are made from a Tungsten (also called Wolfram) wire heated at between 2500 and 3500 K by passing an electric current through it). The glass bulb enclosing it helps maintain the temperature and the low pressure inert gases filling it help slow down the evaporation of the metal (which can be seen in old lamps as a blackish deposit on the inside of glass bulb surface). These lamps produce a continuous spectrum (without well defined emission peaks), close to that from a true black body at the same temperature. Lamps with certain types of built-in reflectors may display a somewhat distorted spectrum as a result of interference or because of wavelength-selective properties (e.g. it is not unusual for lamps to have a reflector with high reflectivity for visible radiation but relatively high transmisivity for infra-red radiation).

Carbon arc lamps produce light by means of an electric "arc" between two carbon electrodes, the arc heats the electrodes and carbon evaporates and because of its high temperature in-between the electrodes inducing light emission. The spectrum is broad but rather different to sunlight. Carbon arc lamps can be very bright and used in cinema projectors. They were invented before the incandescent tungsten lamp. Xenon arc lamps use Xenon gas enclosed in a special glass bulb. Xenon arc lamps have an emission spectrum rather similar to that of solar radiation, and together with UV-absorbing filters are frequently

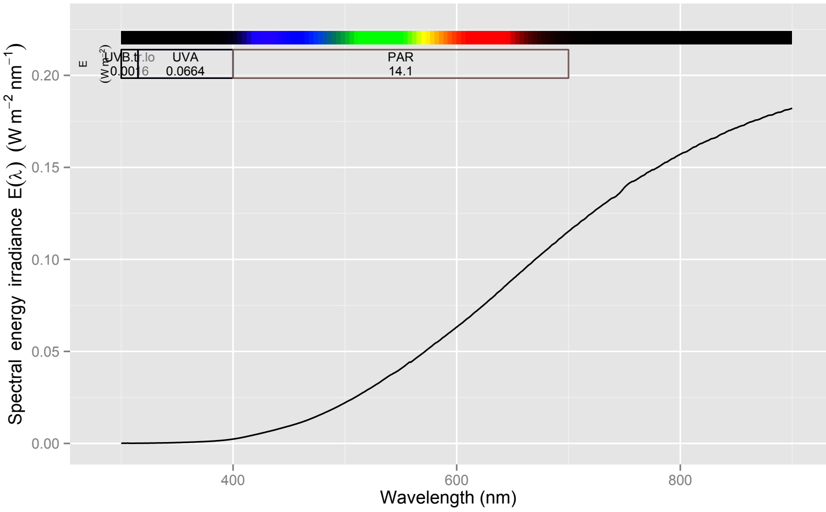


Figure 1.14: Spectral irradiance for a 60 W incandescent lamp

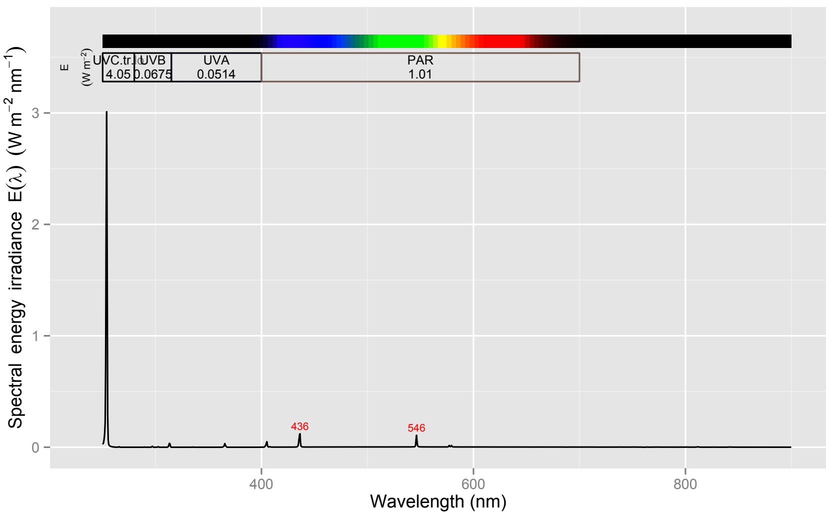


Figure 1.15: Spectral irradiance for a 'germicidal' low pressure mercury lamp.

used in solar simulators. Some Xenon lamps do not emit continuously, such as modern "electronic" flashes used in photographic cameras. In such lamps the flash is produced by slowly charging a capacitor at a high voltage, and subsequently using this electrical charge to generate a short-lived arc in the lamp. Flash duration varies, but can be as short 0.1 ms in flashes used by photographers.

Other gas-discharge lamps use other gases or "vapours" or mixes of them. In these lamps, the elemental emission lines (corresponding to transitions between

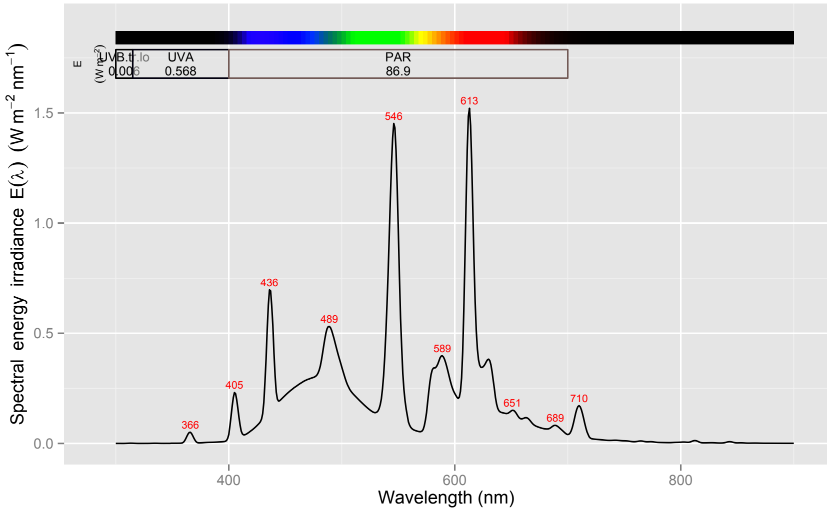


Figure 1.16: Spectral irradiance for a 'daylight', approx. 5200 K, fluorescent tube (Philips 36W 950).

allowed energy states) are very well defined as long as the glass ampoule is not coated with special fluorescent compounds, and in many cases can be used as wavelength standards for calibration of spectrometers. The low pressure sodium lamps, easily recognizable by the orange light they emit, emit the same orange colour as that emitted by the flame of a gas ring in a cooker when water containing salt boils over from a pot. Low pressure mercury "vapour" lamps, such as germicidal ones made with an un-coated quartz-glass tube (technically called envelope) emit clearly at the know emission lines of mercury (Fig. 1.15). Being the container UV and VIS transmitting the strong line at 253.xx nm is very active as a germicidal agent. The "normal" fluorescent tubes used for illumination are enclosed in a tube coated with a so-called "phosphor" which absorbs UV radiation and re-emits it as visible radiation (Fig. 1.16). The spectrum of the emitted radiation is a combination of radiation emitted by the gaseous mercury, in particular those lines in the VIS region and to some extent in the UVA region, together with visible radiation re-emitted by the coating.

A more recent development is light generated by solid-state semiconductor devices or light-emitting diodes, once again light emission is the result of a transition between energy states of matter, but although emission takes place as a single peak, the peak is not as narrow or well defined as for elemental emission lines in discharge lamps (Fig. 1.17). Emission peaks have usually HFW of between 10 and 30 nm and their central wavelength may slightly shift depending on temperature and electrical current flowing through them. True LEDs always have a single peak of emission. White LEDs are based on a similar idea to that of fluorescent lamps: blue (or in some cases UVA) emitting LEDs are combined with a "phosphor" which absorbs in part the emitted radiation and re-emits the energy as radiation at longer wavelengths (Fig. 1.18). In some designs the phosphor is coated close to the semiconductor die, but in other cases,

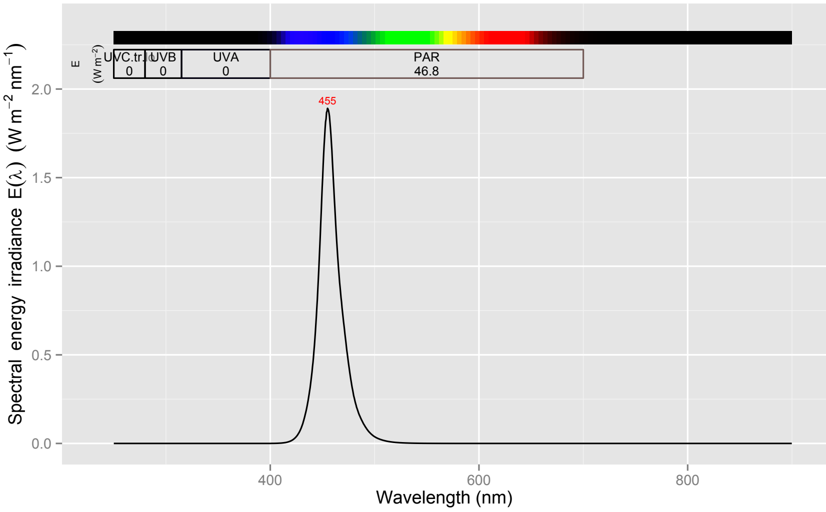


Figure 1.17: Spectral irradiance for a blue LED array (Huey Jann, 50 W).

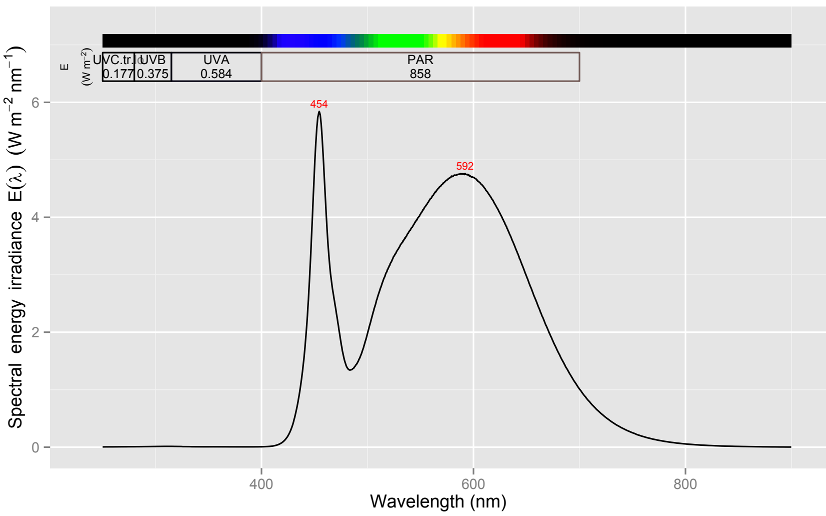


Figure 1.18: Spectral irradiance for 'neutral white LED', 4000 K, array (Lumitronix SmartArray Q36 LED-Module, 39W, using Nichia 757 LEDs).

especially some arrays, the phosphor is in or on the encapsulating polymer.

Finally lasers, are different in that a laser is not another type of primary source of radiation. Lasing is a phenomenon which allows the generation of coherent radiation from a beam of incoherent radiation by means of a "cavity". Different primary sources of radiation can be used in lasers. In the case of laser diodes, an LED is the primary source of radiation. There are different possible types of cavities, for example gas-filled or solid state. Lasers are pulsed light sources, they do not emit continuously, although in many cases the frequency at which pulses are produced can be high. Even though laser pointers and other readily available lasers seem to us as being a continuous source of radiation, they are not. In fact, they are pulsed, and the duty cycle is low (pulses are brief compared to 'gaps') but each pulse has high energy. As radiation is in addition in a very narrow beam and almost of a single wavelength, a laser delivers spatially and temporarily concentrated energy pulses, that can make the beam from a 1 mW laser pointer easily visible at a distance of tens of meters in a lecture hall illuminated with lamps emitting in total hundreds of watts of visible radiation. For the same reason, even lasers emitting as little 1 mW if pointed directly into the eyes can cause permanent eye-sight damage.

1.5 Absorption and reflection of radiation

Authors' note: *We need to explain here the physics of absorption and reflection from the point of view of optical properties. Photochemistry will be introduced in a separate chapter.*

1.6 Radiation interactions in tissues and cells

1.7 Radiation interactions in plant canopies

The attenuation of visible and UV radiation by canopies is difficult to describe mathematically because it is a complex phenomenon. The spatial distribution of leaves is in most cases not uniform, the display angle of the leaves is not random, and may change with depth in the canopy, and even in some cases with time-of-day. Here we give only a description of the simplest approach, the use of an approximation based on Beer's law as modified by (Monsi and Saeki 1953), reviewed by (Hirose 2005). Beer's law (Equation 1.8) assumes a homogeneous light absorbing medium such as a solution. However, a canopy is heterogenous, with discrete light absorbing objects (the leaves and stems) distributed in a transparent medium (air).

$$I_z = I_0 \cdot \mathrm{e}^{-K\,L_z} \tag{1.16}$$

Equation 1.16 describes the radiation attenuated as a function of leaf area index (L or LAI) at a given canopy depth (z). The equation does not explicitly account for the effects of the statistical spatial distribution of leaves and the effects of changing incidence angle of the radiation. Consequently, the empirical extinction coefficient (K) obtained may vary depending on these factors. K is not only a function of plant species (through leaf optical properties, and how leaves are displayed), but also of time-of-day, and season-of-year—as a consequence of solar zenith angle—and degree of scattering of the incident radiation. As the degree of scattering depends on clouds, and also on wavelength, the extinction coefficient is different for UV and visible radiation. Radiation extinction in canopies has yet to be studied in detail with respect to UV radiation, mainly because of difficulties in the measurement of UV radiation compared to PAR, a spectral region which has been extensively studied.

Ultraviolet radiation is strongly absorbed by plant surfaces, although cuticular waxes and pubescence on leaves can sometimes increase UV reflectance. The diffuse component of UV radiation is larger than that of visible light (Figure 1.11). In sunlit patches in forest gaps the diffuse radiation percentage is lower than in open areas, because direct radiation is not attenuated but part of the sky is occluded by the surrounding forest. Attenuation with canopy depth is on average usually more gradual for UV than for PAR. The UV irradiance decreases with depth in tree canopies, but the UV:PAR ratio tends to increase (see Brown et al. 1994). In contrast, (Deckmyn et al. 2001) observed a decrease in UV:PAR ratio in white clover canopies with planophyle leaves. (Allen et al. 1975) modelled the UV-B penetration in plant canopies, under normal and depleted ozone conditions. (Parisi and Wong 1996) measured UV-B doses within model plant canopies using dosimeters. The position of leaves affects UV-B exposure, and it has been observed that heliotropism can moderate exposure and could be a factor contributing to differences in tolerance among crop cultivars (Grant 1998, 1999a,b, 2004).

Detailed accounts of different models describing the interaction of radiation and plant canopies, taking into account the properties of foliage, are given by (Campbell and Norman 1998) and (Monteith and Unsworth 2008).

1.8 Radiation interactions in water bodies

Authors' note: *Andreas, could you be the lead author of this section?*

CHAPTER 2

Quantification and spectroscopy

Abstract

In this chapter we explain the basis of spectral measurements, including radiation spectra, transmission and reflectance spectra.

2.1 Radiation and molecules

2.1.1 Fluorescence

2.1.2 Phosphorescence

2.2 Surface phenomena

2.2.1 Refraction

2.2.2 Difraction

2.3 Geometrical considerations

2.3.1 Scatering

2.3.2 Angle of incidence

2.4 Measured quantities

2.4.1 Irradiance, radiance, and fluence

2.4.2 Specular and total reflectance

2.4.3 Internal and total transmittance

2.4.4 Absorbance and transmittance

CHAPTER 3

Photochemistry

Abstract

In this chapter we explain how UV and VIS radiation can drive chemical reactions, both in inorganic and organic molecules, both *in vitro* and within living organisms. We also describe how action- and response spectra are measured.

3.1 Light driven reactions

3.2 Silver salts and photographic films

3.3 Bleaching by UV radiation

3.4 Chlorophyll

3.5 Plant photoreceptors

3.6 Animal photoreceptors

3.7 Action spectroscopy

3.8 Photoreception tuning

Part II

Tools used for calculations

CHAPTER 4

Software

Abstract

In this chapter we describe the software we used to run the code examples and typeset this handbook, and how to install it. Which is basically the same we use for everyday data analysis and typesetting.h

4.1 Introduction

The software used for typesetting this handbook and developing the r4photobiology suite is free and open source. All of it is available for the most common operating systems (Unix including OS X, Linux and its variants, and Windows). It is also possible to run everything described here on a Linux server running the server version of RStudio, and access the server through a web browser.

For just running the examples in the handbook, you would need only to have R installed. That would be enough as long as you also have a text editor available. This is possible, but does not give a very smooth workflow for data analyses which are beyond the very simple. The next stage is to use a text editor which integrates to some extent with R, but still this is not ideal, specially for writing packages or long scripts. Currently the best option is to use the integrated development environment (IDE) called 'RStudio'. This is an editor, but tightly integrated with R. Its advantages are especially noticeable in the case of errors and 'debugging'. During the development of the packages, we used RStudio exclusively.

The typesetting is done with LaTeX and the source of this handbook was edited using both the shareware editor WinEdt (which excels as a LaTeX editor) and RStudio which is better suited to the debugging of the code examples. We also used LaTeX for our first handbook (Aphalo, Albert, Björn, Ylianttila et al. 2012).

Combining R with Markdown (Rmarkdown: Rmd files) or LaTeX (Rnw fiels) to produce *literate* scripts is best for reproducible research and our suite of packages is well suited for this approach to data analysis. However, it is not required to go this far to be able to profit from R and our suite for simple analyses, but the set up we will describe here, is what we currently use, and it is by far the best one we have encountered in 18 years of using and teaching how to use R.

We will not give software installation instructions in this handbook, but will keep a web page with up-to-date instructions. In the following sections we briefly describe the different components of a full and comfortable working environment, but there are many alternatives and the only piece that you cannot replace is R itself.

4.2 The different pieces

4.2.1 R

You will not be able to profit from this handbook's 'Cook Book' part, unless you have access to R. R (also called Gnu S) is both the name of a software system, and a dialect of the language S. The language S, although designed with data analysis and statistics in mind, is a computer language that is very powerful in its own way. It allows object oriented programming. Being based on a programming language, and being able to call and being called by programs and subroutine libraries written in several other programming languages, makes R easily extensible.

R has a well defined mechanism for "add-ons" called packages, that are kept in the computer where R is running, in disk folders that conform the library. There is a standard mechanism for installing packages, that works across operating systems (OSs) and computer architectures. There is also a Comprehensive R Archive Network (CRAN) where publicly released versions of packages are kept. Packages can be installed and updated from CRAN and similar repositories directly from within R.

The *engine* behind the production of the pages of this handbook is the R package `knitr` which allows almost seamless integration of R code and text marked up using LaTeX. We have used in addition several other packages, both by using them as building blocks in our packages, and for the production of the examples. The most notable ones are: `data.table`, `lubridate`, and `ggplot2`. Packages `devtools` and `testthat` significantly easied the task of package development and coding.

If you are not familiar with R, please, go through the separately available Supplements **??**, **??**, **??**, and **??**, and/or learn from some of the books listed in Appendix **??**, before delving into our 'Cook Book'.

4.2.2 RStudio

RStudio exists in two versions with identical user interface: a desktop version and a server version. The server version can be used remotely through a web browser. It can be run in the 'cloud', for example, as an AWS instance

(Amazon Web Services) quite easily and cheaply, or on one's own server hardware. RStudio is under active development, and constantly improved (visit `http://www.rstudio.org/` for an up-to-date description and download and installation instructions.

4.2.3 Version control: Git and Subversion

Version control systems help by keeping track of the history of software development, data analysis, or even manuscript writing. They make it possible for several programmers, data analysts, authors and or editors to work on the same files in parallel and then merge their edits. They also allow easy transfer of whole 'projects' between computers. Git is very popular, and Github and Bitbucket are popular hosts for repositories. Git itself is free software, was designed by Linus Tordvals of Linux fame, and can be also run locally, or as one's own private server, either as an AWS instance or on other hosting service, or on your own hardware.

4.2.4 C++ compiler

Although R is an interpreted language, a few functions in our suite are written in C++ to achieve better performance. On OS X and Windows, the normal practice is to install binary packages, which are ready compiled. In other systems like Linux and Unix it is the normal practice to install source packages that are compiled at the time of installation. With suitable build tools (e.g. RTools for Windows) source packages can be installed and developed in any of the operating systems on which R runs.

4.2.5 LaTeX

LaTeX is built on top of TeX. TeX code and features were 'frozen' (only bugs are fixed) long ago. There are currently a few 'improved' derivatives: pdfTeX, XeTeX, and LuaTeX. Currently the most popular TeX in western countries is pdftex which can directly output PDF files. XeTeX can handle text both written from left to right and right to left, even in the same document and additional font forats, and is the most popular TeX engine in China and other Asian countries.

For the typesetting of this handbook we used several LaTeX packages, of which those that most affected appearance are `memoir`, `hyperref`, `booktabs`, `pgf/tikz` and `biblatex`. The TeX distribution we used is MikTeX.

4.2.6 Markdown

Markdown is a simple markup language, which although offering somehow less flexibility that LaTeX is much easier to learn and which can be easily converted to various different output formats in addition to PDF.

CHAPTER 5

Photobiology R packages

Abstract

In this chapter we describe the suite of R packages for photobiological calculations 'r4photobiology', and explain how to install them.

5.1 Expected use and users

The aim of the suite is to both provide a framework for teaching VIS and UV radiation physics and photobiology through a set of functions and data examples. Furthermore, we expect these functions and data to be useful for active researchers during design of experiments, data analysis and data validation. In particular we hope the large set of example data will make it easy to carry out sanity checks of newly acquired and/or published data.

Given the expected audience of both students and biologists, rather than data analysts, or experienced programmers, we have aimed at designing a consistent and easy to understand paradigm for the analysis of spectral data. The design is based on our own user experience, and on feedback from our students and 'early adopters'.

5.2 The design of the framework

The design of the 'high level' interface is based on the idea of achieving simplicity of use by hiding the computational difficulties and exposing objects, functions and operators that map directly to physical concepts. Computations and plotting of spectral data centers on two types of objects: *spectra* and *wavebands* (Figure 5.1). Al spectra have in common that observations are referenced to a wavelength value. However, there are different types spectral objects, e.g. for light sources and responses to light. Waveband objects include much more

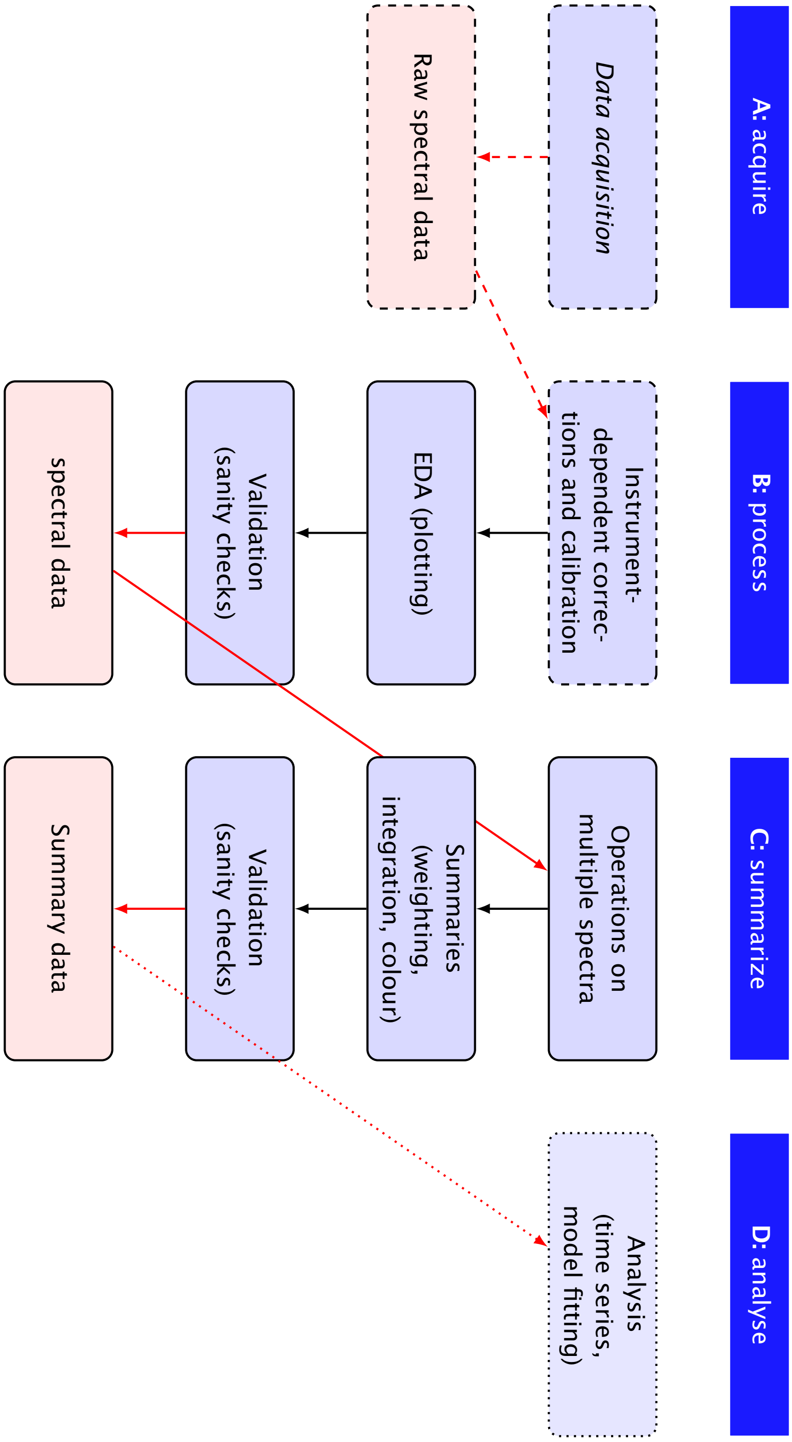


Figure 5.1: Data "pipeline" from acquisition to analysis of spectral data

Box 5.1: Elements of the framework used by all packages in the suite.

`_spct` Spectral objects are containers for different types of spectral data, data which is referenced to wavelength. These data normally originate in measurements or simulation with models.

`_multi_spct` Containers for spectral objects are used to store related spectral objects, such as time series of spectral objects or spectral images.

`wavebands` Waveband objects are containers of 'instructions' for the quantification of spectral data. In addition to the everyday definition as a range of wavelengths, we include the spectral weighting functions used in the calculation of what are frequently called weighted or effective exposures and doses.

summary functions Different summary functions return different quantities through integration over wavelengths and take as arguments spectra and wavebands.

maths operators and functions Are used to combine and/or transform spectral data, and in some cases to apply weights defined by wavebands.

than information about a range of wavelengths, they can also include information about a transformation of the spectral data, like a biological spectral weighting function (BSWF). In addition to functions for calculating summary quantities like irradiance from spectral irradiance, the packages define operators for spectra and wavebands. The use of operators simplifies the syntax and makes the interface easier to use.

A consistent naming scheme as well as consistency in the order of function arguments across the suite.... Data objects are *tidy* as defined by in (**Wickham2013**), in other words data on a row always corresponds to a single observation event, although such an observation can consist in more than one measured or derived quantity. Data from different observations are stored in different objects, or if in the same object they are *keyed* using and index variable.

The same summary methods, are available for `_spct` and `_multi_spct`, in the first case returning a vector, and in the second case, a `data.frame` object.

Package `photobiology` can be thought as a framework defining a way of storing spectral data plus 'pieces' from which specific summaries can be constructed. Extensibility and reuse is at the core of the design. This is achieved by using the weakest possible assumptions or expectations about data properties and avoiding as much as possible the hard-coding of any constants or size limits. This, of course, has a cost in possibly slower execution speed.

Within these constraints an effort has been made to remove performance bottleneck by means of C++ code and passing data objects by reference when possible.

```
e_irrad(sun.spct * polyester.new.spct, CIE())
```

Is all what is needed to obtain the CIE98-weigthed energy irradiance simulating the effect of a polyester filter on the example solar spectrum, which of course, can be substituted by other spectral irradiance and filter data.

When we say that we hide the computational difficulties what we mean, is that in the example above, the data for the two spectra do not need to be available at the same wavelengths values, and the BSWF is defined as a function. Interpolation of the spectral data and calculation of spectral weighting factors takes place automatically and invisibly. All functions and operators function without error with spectra with varying (even arbitrarily and randomly varying) wavelength steps. Integration is always used rather than summation for summarizing the spectral data.

There is a lower layer of functions, used internally, but also exported, which allow improved performance at the expense of more complex scripts and commands. This user interface is not meant for the casual user, but for the user who has to analyse thousands of spectra and uses scripts for this. For such users performance is the main concern rather than easy of use and easy to remember syntax. Also these functions handle any wavelength mismatch by interpolation before applying operations or functions.

The suite also includes data for the users to try options and ideas, and helper functions for plotting spectra using other R packages available from CRAN, in particular `ggplot2`. There are some packages, not part of the suite itself, for data acquisition from Ocean Optics spectrometers, and application of special calibration and correction procedures to those data. A future package will provide an interface to the TUV model to allow easy simulation of the solar spectrum.

5.3 The suite

The suite consists in several packages. The main package is `photobiology` which contains all the generally useful functions, including many used in the other, more specialized, packages (Table 5.1).

Spectral irradiance objects (class `source_spct`) and spectral response/action objects (class `response_spct`) can be constructed using energy- or photon-based data, but this does not affect their behaviour. The same flexibility applies to spectral transmittance vs. spectral absorbance for classes `filter_spct`, `reflector_spct` and `object_spct`.

Although by default low-level functions expect spectral data on energy units, this is just a default that can be changed by setting the parameter `unit.in = "photon"`. Across all data sets and functions wavelength vectors have name `w.length`, spectral (energy) irradiance `s.e.irrad`, photon spectral irradiance `s.q.irrad`[1], absorbance ($\log_{10}$-based) A, transmittance (fraction of one)

[1] `q` derives from ‘quantum’.

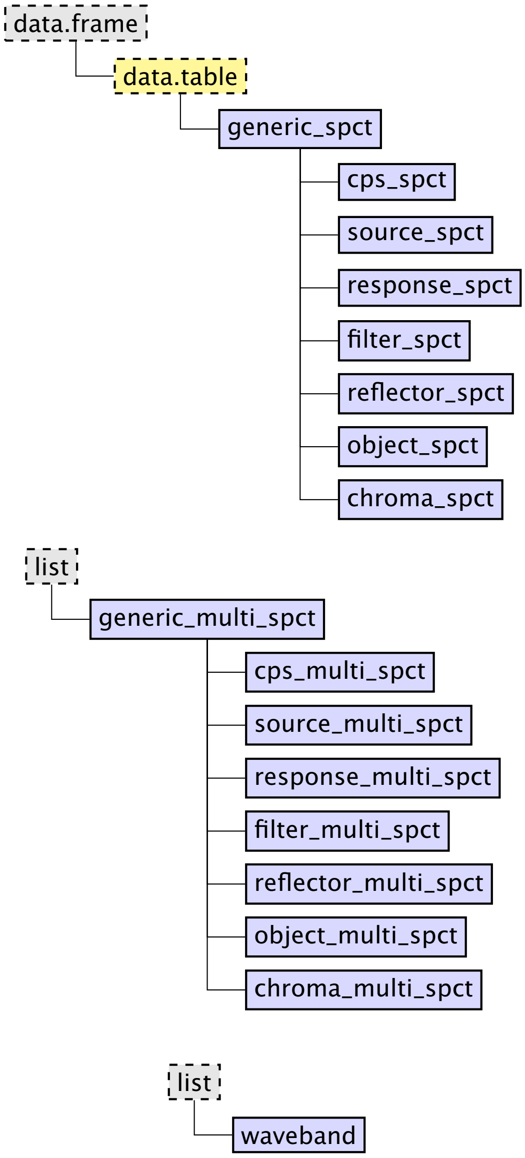


Figure 5.2: Object classes used in the packages. Objects of `_spct` classes are used to store spectra, in most cases a single spectrum. Objects of `_multi_spct` classes can be used to store *collections* of `_spct` objects, in most cases all belonging to the same class. Objects of class `waveband` contain information used for quantification: boundaries of a wavelength range and, optionally, spectral weighting functions. Gray-filled boxes represent classes defined in base R, yellow-filled boxes represent classes defined by contributed packages available through CRAN, Comprehensive R Archive Network, and blue-filled boxes represent classes defined in package photobiology.

Table 5.1: Packages in the r4photobiology suite. Packages not yet released are highlighted with a red bullet •, and those at 'beta' stage with a yellow bullet •, those relatively stable with a green bullet •.

	Package	Type	Contents
•	photobiologyAll	dummy	loads other packages of the suite
•	photobiology	funs + classes	basic functions, class definitions, class methods and example data
•	photobiologyInOut	functions	data import/export functions
•	photobiologyWavebands	definitions	quantification of radiation
•	photobiologygg	functions	extensions to package `ggplot2`
•	photobiologySun	data	spectral data for solar radiation
•	photobiologyLamps	data	spectral data for lamps
•	photobiologyLEDs	data	spectral data for LEDs
•	photobiologyFilters	data	transmittance data for filters
•	photobiologySensors	data	response data for sensors
•	photobiologyReflectors	data	reflectance data for materials
•	photobiologyPlants	funs + data	photobiology of plants
•	rOmniDriver	functions	Ocean Optics spectrometers
•	MayaCalc	functions	UV and VIS irradiance data processing for Maya2000 Pro
•	rTUV	funs + data	TUV model interface

`Tfr`, transmittance (%) `Tpc`, reflectance (fraction of one) `Rfr`, reflectance (%) `Rpc`, and absorptance (fraction of one) `Afr`.

Wavelengths should always be in naanometres (nm), and when conversion between energy and photon based units takes place no scaling factor is used (an input in $\mathrm{W\,m^{-2}\,nm^{-1}}$ yields an output in $\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ rather than $\mathrm{\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}}$).

The suite is still under active development. Even those packages marked as 'stable' are likely to acquire new functionality. By stability, we mean that we hope to be able to make most changes backwards compatible, in other words, we hope they will not break existing user code.

5.4 The r4photobiology repository

I have created a repository for the packages. This repository follows the CRAN folder structure, so package installation can be done using normal R commands. This means that dependencies are installed automatically and that automatic updates are possible. The build most suitable for the current system and R version is also picked automatically if available. It is normally recommended that you do installs and updates on a clean R session (just after starting R or RStudio). For easy installation and updates of packages, the r4photobiology repository can be added to the list of repositories that R knows about.

Whether you use RStudio or not it is possible to add the r4photobiology repository to the current session as follows, which will give you a menu of additional repositories to activate:

```
setRepositories(
  graphics = getOption("menu.graphics"),
  ind = NULL,
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

If you know the indexes in the menu you can use this code, where '1' and '6' are the entries in the menu in the command above.

```
setRepositories(
  graphics = getOption("menu.graphics"),
  ind = c(1, 6),
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

Be careful not to issue this command more than once per R session, otherwise the list of repositories gets corrupted by having two repositories with the same name.

Easiest is to create a text file and name it '`.Rprofile`', unless it already exists. The commands above (and any others you would like to run at R start up) should be included, but with the addition that the package names for the functions need to be prepended. So previous example becomes:

```
utils::setRepositories(
  graphics = getOption("menu.graphics"),
  ind = c(1, 6),
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

The `.Rprofile` file located in the current folder is sourced at R start up. It is also possible to have such a file affecting all of the user's R sessions, but its location is operating system dependent, it is in most cases what the OS considers the current user's *HOME* directory or folder (e.g. 'My Documents' in recent versions of MS-Windows). If you are using RStudio, after setting up this file, installation and updating of the packages in the suite can take place exactly as for any other package archived at CRAN.

The commands and examples below can be used at the R prompt and in scripts whether RStudio is used or not.

After adding the repository to the session, it will appear in the menu when executing this command:

```
setRepositories()
```

and can be enabled and disabled.

In RStudio, after adding the r4photobiology repository as shown above, the photobiology packages can be installed and uninstalled through the normal RStudio menus and dialogues, and will listed after typing the first few characters of their names. For example when you type 'photob' in the packages field, all the packages with names starting with 'photob' will be listed.

They can be also installed at the R command prompt with the following command:

```
install.packages(c("photobiologyAll", "photobiologygg"))
```

and updated with:

```
update.packages()
```

The added repository will persist only during the current R session. Adding it permanently requires editing the R configuration file, as discussed above. Take into consideration that `.Rprofile` is read by R itself, and will take effect whether you use RStudio or not. It is possible to have an user-account wide .Rprofile file, and a different one on those folders needing different settings. Many other R options can also be modified by means of commands in the .Rprofile file.

Part III

Cookbook of calculations

Part IV

Data acquisition and modelling

Part V

Catalogue of example data

Part VI

Optimizing computation speed

Authors' note: *Chapter not included as example code is giving errors at the moment.*

CHAPTER 6

Further reading

6.1 Radiation physics

6.2 Photochemistry

6.3 Photobiology

6.4 Using R

6.5 Programming in R

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Glossary

absorbance $A = \log E_0/E_1$, where E_0 is the incident irradiance, and E_1 is the transmitted irradiance. ix

absorptance radiation that is absorbed by an object, as a fraction of the incident irradiance: $\alpha = E_{\mathrm{abs}}/E_0$, where E_0 is the incident irradiance and E_{abs} is the absorbed irradiance. ix

biological spectral weighting function a function used to estimate the biological effect of radiation. It is convoluted—i.e. multiplied wavelength by wavelength—with the spectral irradiance of a source of UV radiation to obtain a biologically effective irradiance. ix

CRAN, Comprehensive R Archive Network A network of software and documentation repositories for R packages and R itself. 41

direct radiation solar radiation that arrives directly at the ground level, without being scattered by gases and particles of the atmosphere. 16, 25

global radiation total solar radiation arriving at ground level. It is the sum of direct and diffuse radiation. 16, *see* direct radiation

isotropic radiation is isotropic when it arrives equally from all directions, e.g. it is completely diffuse. *see* scattered or 'diffuse' radiation

photosynthetic photon flux density another name for 'PAR photon irradiance'. x

photosynthetically active radiation radiation driving photosynthesis in higher plants, it describes a wavelength range—i.e. λ =400–700 nm—but does not define whether an energy or photon quantity is being used. x

proportional-integral-derivative a *proportional integral derivative* controller (PID controller) is a control loop feedback mechanism. A PID controller calculates an "error" value as the difference between a measured process variable and a desired setpoint. The controller attempts to minimize the error by adjusting the process control inputs. A well tuned PID controller (with correct parameters) minimizes overshoot and transient deviations, by adjusting, for example, the dimming in a modulated system based on the size of the error and the response characteristics of the controlled system. x

radiation amplification factor gives the percent change in biologically effective UV irradiance for a 1% change in stratospheric ozone column thickness. Its value varies with the BSWF used in the calculation. x

reflectance radiation that is reflected by an object, as a fraction of the incident irradiance: $\rho = E_{\mathrm{rfl}}/E_0$, where E_0 is the incident irradiance and E_{rfl} is the reflected irradiance. ix

scattered or 'diffuse' radiation solar radiation that arrives at ground level after being scattered by gases and particles of the atmosphere, also called 'diffuse radiation'. 16

transmittance radiation that is transmitted by an object, as a fraction of the incident irradiance: $\tau = E_{\mathrm{trs}}/E_0$, where E_0 is the incident irradiance and E_{trs} is the transmitted irradiance. ix

Index

Part VII

Appendix

APPENDIX A

Build information

```
Sys.info()

##                        sysname
##                      "Windows"
##                        release
##                        "7 x64"
##                        version
## "build 7601, Service Pack 1"
##                       nodename
##                        "MUSTI"
##                        machine
##                       "x86-64"
##                          login
##                       "aphalo"
##                           user
##                       "aphalo"
##                 effective_user
##                       "aphalo"
```

```
sessionInfo()

## R version 3.2.1 (2015-06-18)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 7 x64 (build 7601) Service Pack 1
##
## locale:
## [1] LC_COLLATE=English_United Kingdom.1252
## [2] LC_CTYPE=English_United Kingdom.1252
## [3] LC_MONETARY=English_United Kingdom.1252
## [4] LC_NUMERIC=C
## [5] LC_TIME=English_United Kingdom.1252
##
## attached base packages:
## [1] methods   tools     stats     graphics
```

```
## [5] grDevices utils     datasets  base
##
## other attached packages:
##  [1] photobiologyLEDs_0.3.0
##  [2] photobiologyLamps_0.3.1
##  [3] photobiologySun_0.3.2
##  [4] photobiologygg_0.3.5
##  [5] scales_0.2.5
##  [6] ggplot2_1.0.1
##  [7] proto_0.3-10
##  [8] photobiologyWavebands_0.3.1
##  [9] photobiology_0.7.0
## [10] data.table_1.9.4
## [11] stringr_1.0.0
## [12] knitr_1.10.5
##
## loaded via a namespace (and not attached):
##  [1] Rcpp_0.11.6      magrittr_1.5
##  [3] MASS_7.3-42      munsell_0.4.2
##  [5] colorspace_1.2-6 splus2R_1.2-0
##  [7] highr_0.5        plyr_1.8.3
##  [9] caTools_1.17.1   grid_3.2.1
## [11] gtable_0.1.2     digest_0.6.8
## [13] reshape2_1.4.1   formatR_1.2
## [15] bitops_1.0-6     memoise_0.2.1
## [17] evaluate_0.7     labeling_0.3
## [19] stringi_0.5-5    lubridate_1.3.3
## [21] chron_2.3-47
```