A simulation tool for the spectroscopic calibration of atmospheric transmission for LSST

Reference Document Part I –Version 2.

APC/LSST Technical Note

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WARNING : This is a working document not fit for publication, it is produced for internal use inside the LSST Calsim collaboration. Some full subsections have been copied and glued from other documents.

The complete document is made of two part

Part I (this) : Presentation

Part II (to appear) : Software Guide

Contents of Part I

1. Introduction

The so called *Atmosphere Simulator* described here was developed for the purpose of testing and optimizing the LSST Calibration procedure. The current document ambitions to provide potential users (or future modifiers) with the information they need to understand the data and the processes they use. The document is made of two parts. Part I (this), is dedicated to a description of the processes and resulting data. Part II (to appear soon (hopefully)) is a user guide to the software modules developed in this frame. Only after several iterations with the calibration actors will this document reach a state approaching this ambition. In this introduction we remind the mission(s) assigned to the simulator and give a first presentation of its main building blocks. In section 2 we describe the exploratory phase of this work that is discovering how to get the proper combination of Modtran parameters that drives the atmosphere in the state you need. In section 3, we explain the concept of "atmospheric scenario" that is how we start from a list of heuristic statements describing the evolution of the local weather in as much as it affects light transmission, to produce series of atmosphere parameters for long periods of time and from them to atmosphere transmission spectra. And we present a series of photometric statistics illustrating the impact of atmospheric effects and their variability on the photometry of astronomical objects.

1.1 The role of atmosphere simulations in the LSST Calsim project.

High-priority science goals of the LSST mission such as weak lensing and baryon acoustic oscillations require exquisite knowledge of the density and spatial distribution of galaxies. The atmosphere can introduce photometric errors correlated on spatial scales of tens of arc-minutes where much of the power in these analyses is to be found. The LSST SRD includes a design specification of 10 milli - magnitude on the rms variation of the photometric zero-point across the sky, but this has been strengthened to require that errors of this magnitude not be spatially correlated. The stretch goal and the target for residual errors induced by the atmosphere is 5 milli - mag.

The calibration plan includes auxiliary hardware to measure atmospheric transparency contemporaneously with LSST science observations. A robotic auxiliary telescope (AT) will be used to monitor the spectral dependence of atmospheric transparency and measure atmospheric extinction. Together with the celestial sentinel stars in each LSST FOV, these measurements will provide determination of the magnitude and spatial structure of atmospheric transparency across the LSST FOV and optical bandpass at the times science data are taken.

1.1.1 Simulating Atmospheric effects relevant to the calibration process

The calibration process must be robust to a broad variety of atmospheric conditions, including those prevailing during nights traditionally classified by astronomers as non photometric. This implies extensive simulations based on atmosphere transmission spectra reproducing the complexity of the real atmosphere with all its constituents and their variations in space and time, in so far as they affect light transmission. The development of this simulation tool pompously baptised ***"Atmosphere simulator***" in the following involved the construction of increasingly complex and realistic atmosphere change scenarios expressed as a series of parameters describing the molecular and particular content of the atmosphere column along every observing line of sight. These parameters are then converted to atmospheric transmission spectra via the Modtran atmosphere radiative transport code.

We essentially rely upon Modtran for understanding and calculating the physics of what happens to light while it crosses the atmospheric layer down to the telescope and focus on the task of feeding this computation with a broad variety of meteorological scenarios governing variations of the atmosphere components that contribute to the three major effects: Rayleigh diffusion, Mie diffusion generated by aerosols and molecular diffusion. These meteorological scenarios must match two different requirements: for one thing they ought to sample the whole diversity of accidents likely to affect the astrophysical signal so as to serve as a bench test to the calibration process. For the other thing they ought to mimic situations as close as possible from those that those likely to prevail during LSST operations. Including the amplitudes and frequency of phenomena (which orders of magnitudes may affect the performance of calibration algorithms) and including also seasonal effects that may create on the long range dangerous systematics affecting in particular cosmological results.

One difficulty is the Modtran parameterization: while the physics of the atmosphere as well in terms of presence or abundance of constituents and or thermo-dynamical equilibrium of the vertical structure as that of the molecular properties of each component is in general highly reliable and the results sufficiently documented in the Modtran outputs, the only entry in the code is managed by a very rigid system of "cards" inherited from the early implementations of the model. These cards are read via fixed Modtran formats not easily accessible. Every attempt to introduce more flexibility in the choice implies further immersion in the heart of this very complex machinery. The correspondence between these parameter and the resulting state of the atmosphere although most often briefly documented, but it has not been designed primarily to obtained the effect you are willing to study. Our first task was to domesticate this machinery to make it produce the atmospheres we needed, without redeveloping what had been the collective task of two generations of specialists.

1.1.2 Reduced Parameterization of the atmosphere transmission for calibration purposes

A by-product of the use of Modtran as the main building block of the atmosphere simulator is the possibility to use this model as a tool to parameterize the atmosphere transmission spectrum in the calibration process itself, thus reducing the task of measuring the transmission spectrum to the more affordable task of estimating a very limited number of parameters.

Essentially, our systematic exploration of a broad variety of Modtran parameterizations show that in so far as light transmission is concerned, one coefficient related to the amount of particles contributing to a given diffusion mechanism gives sufficient degrees of freedom to match all situations. We successfully tested the hypothesis that (with the important exception of aerosols) the transmission spectrum of each contributor is a one to one function of just the number of particles along the line of sight. The one to one function was established for each wavelength bin for each important molecular contributor.

Of course, strictly speaking, the validation of this approach is essentially limited to atmospheres that would behave as predicted by Modtran. Extensive observational validation of this still needed. We can however argue that the physics of molecular absorption for constituents like water vapour, ozone or molecular oxygen are well understood and modelled by Modtran, while the more fuzzy thermodynamic equilibrium of the atmosphere does not alter spectral absorption except via the number of molecules. (Thermal ray broadening and convection drifts have negligible effects)

Concerning aerosols, there is the extra difficulty that the transmission spectrum generated by the Mie diffusion depends on the size distribution of particles but the spectrum is smooth and can be approximated numerically via a very small number of extra free parameters.

1.2 Structure of the Atmosphere Simulator

The simulator first produces ***atmospheric scenarios*** based on more or less realistic descriptions of the evolution of the local weather including long term seasonal variations and shorter term fluctuations of each atmosphere component likely to play a significant role in the atmosphere transmission, namely molecular oxygen and nitrogen, ozone, water vapour, aerosols and clouds. The atmospheric scenario outputs are lists of parameter sets computed every other 0.01 day, stored in the Atmosphere-history.dat file. Parameter sets contain all the information required to compute the atmospheric transmission at a given time. There are two such scenarios described in section 3 of this document.

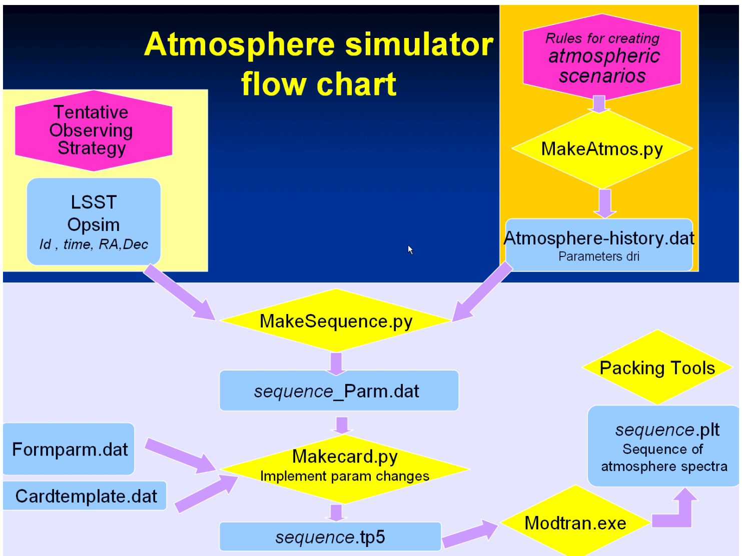


Figure 1.1: Flow chart of the Atmosphere simulation package.

Given the start and end of a calendar period, the ***MakeAtmos*** module translates the adopted meteorological scenario into a **Atmosphere - history** file which is just a list of values of the atmosphere parameters (actually by "atmosphere parameter" we mean the list of Modtran parameters that must be changed in order to match the heuristic description of the atmosphere. All the meteorological knowledge of the simulation should be in this parameter.

Once a history file has been created, the atmosphere transmission can be computed at any time in the period covered by the file, and any direction pointed. The computation is performed by the MODTRAN4 code, a numerical model of the atmosphere developed under the US Air Force which includes all major constituents of the atmosphere under their various physical phases.

The ***MakeSequence*** module, reads a list of telescope pointings specified by time, RA,DEC, picks in the history file the corresponding atmosphere parameters and transforms the whole into parameters that can be interpreted by Modtran.

Eventually the ***Makecard*** module formats the sequence of parameters into a list of "card" sets in the very rigid Modtran input format.

The MakeAtmos part of the process (orange frame in the flow chart) is still in a craftwork state which would be uneasy to export currently. On the contrary, all the content of the pale blue frame could at the cost of a moderate effort be made LSST software compatible and passed to the collaboration so as to permit production of a series of simulations from several Opsim hypotheses, combined with one or two Atmosphere-history files corresponding to one or two pre agreed scenarios.

1.3 Modtran : a summary of the relevant physics of the atmosphere

The MODTRAN numerical model of the atmosphere capitalizes the knowledge accumulated over decades by atmosphere physicists as well as by specialists of remote sensing. This code, developed under the US Air Force, includes all major constituents of the atmosphere under their various physical phases. MODTRAN parameterizes the abundance of these constituents, computes the thermodynamic equilibrium of the resulting atmosphere layer, computes the refraction path of light along upwards or downwards and eventually computes the radiative transfer budget along this path at UV, optical and radio wavelengths. The radiative transfer includes smooth scattering processes by large and intermediate size particles, and molecular processes generating complex band spectra.

1.3.1 What is Modtran

[MODTRAN (Berk et al., 1989; Berk et al., 1998) has served as the U.S. Air Force (USAF) standard moderate spectral resolution radiative transport model for wavelengths extending from the thermal InfraRed (IR) through the visible and into the ultraviolet (0.2 to 10,000.0 □m). The spectroscopy of MODTRAN4 Version 3 Revision 1 (Mod4v3r1) is based on HITRAN2K line compilation (Rothman et al., 1992; Rothman et al., 1998) with update through 2001. The MODTRAN 1 cm-1 statistical band model was developed collaboratively by Spectral Sciences, Inc. and the USAF Research Laboratory, and it provides a fast alternative (100-fold increase in speed) to the USAF first principles and more accurate line-by-line (LBL) radiative transport models, FASCODE (Clough, 1988) and FASCODE for the Environment, FASE (Snell et al., 1995). Comparisons between MODTRAN and FASE spectral transmittances and radiances show agreement to within a few percent or better in the thermal IR. MODTRAN4 includes flux and atmosphere-scattered solar calculations, essential components in analysis of near-IR and visible spectral region data that are not readily generated by LBL models.

Technical descriptions of the MODTRAN approach are available from a variety of sources.

The original MODTRAN 2 code and many of the MODTRAN3 upgrades are described in the 1996 report "MODTRAN 2/3 Report and LOWTRAN 7 Model" (Abreu and Anderson, 1996). The current documentation incorporates material from that report, from Section 3 of the 1988 Users Guide to LOWTRAN 7 (Kneizys et al., 1988), from the 1989 Air Force Research Laboratory (AFRL) report on the MODTRAN band model (Berk et al., 1989), and from the 1996 Spectral Sciences, Inc. report on the cloud and rain model upgrades (Berk and Anderson, 1995).

Articles (Bernstein et al., 1995; Berk et al., 1998) discuss improvements to the band model.][1]

{A MODTRAN4 calculation of atmospheric extinction is shown in Figure 1.1.1. Several processes contribute to the loss of intensity in forward propagating light as it passes through the atmosphere: (1) Rayleigh scattering by molecules that are small compared to the wavelength, (2) Mie scattering by suspended particulate aerosols with sizes comparable to the optical wavelength, and (3) Absorption of light by molecules. In addition to these processes, clouds formed from water droplets and ice crystals with sizes much larger than optical wavelengths will attenuate light, and in the geometric limit, this extinction is "gray", i.e. independent of the wavelength of the light.

The atmospheric optical depth is given by (Lambert-Bouguer-Beer),

$$\tau(\lambda) = \sum_i k_i(\lambda).\rho_i.s \qquad (1.1)$$

The sum is over extinction processes and species, $\boldsymbol{k}$ is the corresponding extinction coefficient, $\boldsymbol{\rho}$ the density of target molecules or particulates, and $\boldsymbol{s}$ is the path length in the atmosphere. The smooth behaviour of the extinction curve seen in Figure B1 is due predominately to Rayleigh-Cabannes and aerosol particulate (Mie) scattering. The extinction coefficients of these two are given by

[1] The section inside [] is copied from Berk , G.P. Anderson , P.K. Acharya, M.L. Hoke , J.H. Chetwynd ,L.S. Bernstein , E.P. Shettle , M.W. Matthew , and S.M. Adler-Golden, 2003, *MODTRAN4 Version 3 Revision 1 USER'S MANUAL*

$$k(\lambda) = a\,\lambda^{-4.05} + b\,\lambda^{-\alpha_p} \qquad (1.2)$$

The spectral index of the particulate scattering α_p depends on the distribution of aerosol sizes and shapes, and is generally between 0.5 and 1.5 (Burki95; Schuster01).}[2]

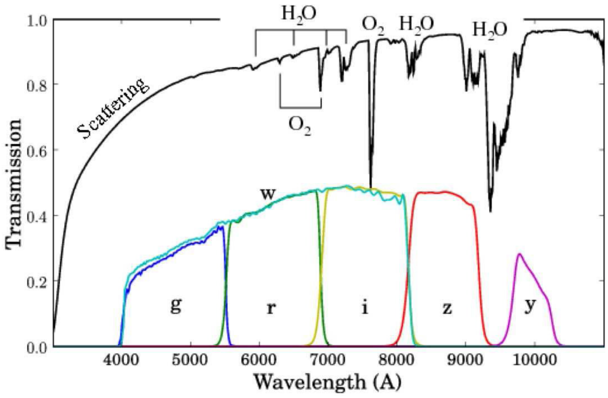


Fig. 1.1.1 Photon transmission through one airmass, with PanSTARRS instrumental sensitivity. This plot shows the different contributions to attenuation of light in passing through the atmosphere, along with filter bands times the expected detector QE, for PanSTARRS. The LSST filter set is similar, but also includes a u band. The atmospheric transmission was computed with MODTRAN for one airmass at an elevation of 10,000 ft (305m), with an initial spectral resolution of 1 cm−1, boxcar smoothed to 1 nm.

1.3.2 Modtran inputs

Modtran includes standard tables and algorithms able to describe as well the equilibrium of the atmosphere constituents as the interaction of main molecules, drops and dusts with lights. It needs input parameters to describe essentially the state of the atmosphere and the observing process of each specific experience or observation. These will be passed by a ***.tp5*** file formated like a variable number of old punched cards following a fixed fortran format.

A MODTRAN "root name" input file provides the full path for MODTRAN I/O. The rootname file must be located in the executable directory and have the name 'modroot.in' or 'MODROOT.IN'.
Modtran will search for the name of the file containing its "card" inputs in a root file named **modroot.in** ; modroot contains a single character string : typically "*cardfile*.tp5".
The name "***cardfile***" is the identifier of a set of Modtran inputs formatted as described in the **Document Modtran_Inputs .**

a) Atmosphere inputs

Atmosphere inputs : atmosphere constituents, temperature and pressure profiles, aerosols and cloud characteristics, plus a number of options that determine the modelling approach.
The fixed characteristics are installed in a Cardtemplate.dat file
The variable ones are the result of an atmospheric scenario produced by the module ***MakeAtmos****…****.py***

Seasonal thermodynamic model

The Modtran parameter MODEL governs a series of options relevant to season and latitude that impacts essentially the gross features of the seasonal effects including the pressure temperature equilibrium. Via pressure, the total amount of oxygen and nitrogen above the observer is obviously affected. Via temperature there are side effects on the water vapour : basically winter air contains less water this can be modulated via the H2O handle (below) but if the water amount is forced into the computation above the saturation point, then Modtran drops the extra water which is not turned into clouds of aerosols (or rain). Clouds and aerosols are modulated independently. There are also typical seasonal values for Ozone. Currently only three standard mid latitude models are used, namely: Mid-latitude summer, mid - latitude winter and US76 (in the Modtran nomenclature).

[2] The section between { } is copied from : LSST Calibration Working Group, Axelrod et al., 2006, *LSST Memorandum (alias White paper).*

Molecules generating the main absorption lines

- H2O water vapour can be modulated with respect to via a specific handle
- O3 ozone can be modulated arbitrarily with respect to the typical season value
- CO2 can be modulated too, but it does not play a major role in our case, having its main effects in the infrared outside the wavelength range of interest
- O2 molecular oxygen produces important absorption line features, but being a dominant constituent in the equilibrium it cannot be modulated by a separate handle.

Aerosol drivers

- IHAZE on/off aerosol switch
- ISEAS season aerosol switch
- IVULC volcanic aerosol type
- IVSA on/off switch for the activation of a specific algorithm for computing the vertical structure of the low aerosol layers in relation with the measure of the atmosphere transparency observed on ground.
- VIS ground meteorological range (km). It is the most flexible handle to play with to drive aerosol variations
- ZAER11 bottom 1rst aerosol layer
- ZAER12 top 1rst aerosol layer
- ZAER21 bottom second aerosol layer
- ZAER22 top second aerosol layer
- SCALE1 SCALE2

Cloud drivers

- ICLD cloud type can introduce a layer of absorbing clouds. There are a number of cloud types in Modtran, however those relevant to astronomical observations are thin layers of Cirrus.
- A separate tool, not in the scope of the present document is currently being developed to simulate small scale random cloud structures generating gray extinction.

b) Observing process inputs

Observing process characteristics are either permanent when related to the Telescope and the required spectral resolution, non permanent characteristics are field and time dependant. The permanent features are telescope altitude longitude and latitude, ground altitude and the adopted spectral range and spectral resolution. They are frozen in the "Cardtemplate.dat file and passed to Modtran by the Make card module. .

Telescope specifications

- Geo - coordinates of the telescope.
longitude L = - 70.749389 ° (70° 44' 57.8 W)
latitude φ = -30.24075° (30° 14' 39.6 S)
- Telescope altitude : 2200 m
- Ground altitude :1500 m . this last parameter plays a role in the computation of the aerosol layers, the adopted value is arbitrary, it was chosen in order to produce the required flexibility in the control of aerosol extinction.

Spectral resolution specifications

The MODTRAN spectra produced since 2007 for the Calsim collaboration are computed in 5212 iso frequency (or energy) bins starting at frequency 9040 cm-1 (1106.1947nm) ending at frequency 35095 cm-1 (284.94087 nm). This is overabundant with regard to the spectra used or envisaged for the auxiliary telescopes (1 nanometre iso wavelength bins). However we decided to keep this high resolution considering that there could impact the photometry of objects with strong S.E.D. gradient. This option will be maintained until there is a conclusive discussion in the collaboration. A rough estimation of the effect of degrading the resolution in terms of magnitude accuracy is shown in table 1.3.1 below. Obviously the error induced by degrading the resolution is not huge, but still an error of 0.0057 in the z filter is not far below the LSST nominal target. It can vary depending on atmospheric conditions and even more so when it comes to considering sources with strong spectral features in the z filter.

Table 1.3.1 : Impact of the adopted spectral resolution on the precision of the magnitude absorbed by one specific atmosphere in the 6 LSST bands using 1) m_0 the $5cm^{-1}$ Modtran iso-frequency bins; 2) m_1 the 1. nm iso-wv bins ; 3) m_2 0.5 nm iso-wv ; 4) m_3 0.25 nm.

Filter	u	g	r	i	z	y
$m_0(5cm^{-1})$	3.467105	1.979556	2.381146	2.719879	3.394813	4.439975
m_1 (1 nm)	3.469039	1.981954	2.384896	2.722594	3.400562	4.442097
$\Delta = m_1 - m_0$	0.001935	-0.002398	-0.003750	-0.002715	**-0.005749**	-0.002121
$\Delta = m_2 - m_0$	-0.000902	-0.001259	-0.001862	-0.001255	-0.002181	-0.001297
$\Delta = m_3 - m_0$	-0.000498	-0.000680	-0.000772	-0.000931	-0.001107	-0.00068

Field specifications

Target sky coordinates and observing time are extracted from simulated catalogs[3] and converted to zenith angle and azimuth at the level of the ***MakeSequence.py*** module in order to

- transfer to Modtran the zenith angle needed for its refraction and radiation transfer computations.
- use the azimuth to alter the VIS driver of aerosol intensity. So as to generate azimuth dependant variations of the aerosol layer

c) Formating inputs to Modtran

Eventually parameter sets gathered by Makesequence are converted to Modtran card sequence by module ***MakeCard.py.*** This module uses two rigidly locked files :

- **Cardtemplate.dat** which is a standard set of Modtran Cards. All the card sets produced by the simulation are build by altering the template set according to the parameter specifications produced by the sequence file.
- **formparm.dat** which specifies the card number of each parameter in the card set its position on the card and the fortran format to write it.

MakeCard eventually produces a ***.tp5*** file containing as many card sets as you need each set leading to a transparency spectrum.

1.3.3 Modtran Outputs.

Standard Modtran 4 outputs.

Modtran returns automatically 6 standard files containing long tables with all details describing the atmosphere characteristics and the absorption spectrum. The most important are ***.tp6, .tp7*** and ***.plt.***

- ***.tp6*** apart from returning an echo of all the input parameters, gives the vertical structure of the column for each molecular and aerosol component. The integrated quantity of each component along the line of sight. Plus the spectrum of the main components. It is of great help to understand the physics.
- ***.tp7*** gives the detailed absorption of each component including those of many minor molecules it is extremely voluminous. And only moderately useful for our purpose.
- ***.plt*** gives the transmission spectrum, i.e. the fraction of energy transmitted at each wavelength.

Reduced Modtran outputs for extensive Calsim atmosphere simulations

A Modtran run for 1000 different atmosphere conditions or lines of sight, generates a 1.9 Gigabytes .tp6 file, a 3.2 G .tp7 and a 0.4 G .plt. Clearly enough, the simulation of spectra for one year of LSST, observations which is order of 300,000 pointings would be a terabyte game if all the outputs are kept. While keeping and compressing one year of .plt files requires only a 20 G. There is no external handle to control the Modtran outputs, so, getting a non verbose version for long term simulations, imposed to enter inside the complex Fortran gas factory.

One weakness of the system is that the .plt file does not keep any memory of the inputs, the only link between the choice of the input parameter set and the outgoing spectrum is provided by the rank of the spectrum in the .plt file is the same as the rank of the card set in the .tp5 file. The rigidity of Fortran I/O structures is actually the only safeguard against mismatching output spectra with input parameters.

[3] Currently there are two tentative simulated LSST pointing catalogues delivered by the collaboration they are known respectively Opsim129 and Opsim3.61. Both cover the same 3 year simulation period. when

2. Atmosphere Model Parameter Control

In this section, we report the results of series of simulations dedicated to checking the link between the assumed properties of the atmosphere at a given time, the Modtran parameters supposed to characterize these properties and the resulting transmission properties. § 2.1 is dedicated to toy tests used essentially as a training set. They are nevertheless useful to understand the role of *seasonal models*. The other subchapters explore and calibrate the handles controlling the main molecular absorbers: water vapour, ozone, molecular oxygen and the more complex role of aerosols. in all cases we check that the absorption spectrum of the absorber is controlled by only one quantity related to the total number of molecules (or aerosol particles) in the atmosphere column crossed by the incident light, although modulating this number in relation with the meteorological situation may require playing with several possibly non trivial keys of the Modtran computation. The dependence of the transmission at each wavelength as a function of this number is shown monotonous but may change drastically from one wavelength to the next depending on optical saturation effects in relation with the details of molecular properties. Modtran is used to establish "growth curves" at each wavelength which open the way to reduce the number of degrees of freedom when it comes to deriving the absorption spectrum from auxiliary telescope observations.

2.1 Exploratory simulation

2.1.1 seasonal models

Figure 2.1.1 shows the spectral transmission at airmass 1.5 under three Modtran seasonal models, zero aerosol assumed (upper left is combined transmission). Two components, water vapour and ozone, are known to be heavily affected seasonal effects : water vapour due to the temperature dependent saturation point, ozone via the summer ozone layer depletion.

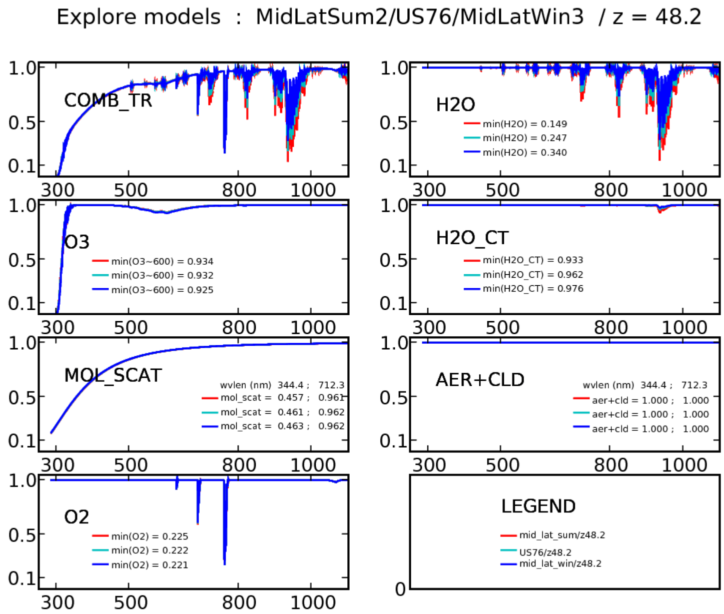


Figure 2.1.1 Spectral transmission at airmass 1.5 under three Modtran seasonal models, spectral contributions for 5 main contributors, upper left is combined transmission (zero aerosol assumed). In order to make small effects readable, a few numerical values at selected wavelengths are overprinted, for line spectra the adopted wavelength is at the minimum of the deepest line, for ozone it is the bottom of the shallow feature around 600 nm. For continuous spectra two arbitrary wavelengths have been selected. *[Spikes above the continuum are spurious plot effects]*.

Modtran implements average seasonal column abundances for these two components and offers free scaling factor parameters (see 2.1.2) to account for larger amplitude variations. Concerning the average seasonal effect, the most visible effect is on water vapour. The ozone column density, as implemented by standard Modtran mid-latitude models, is significantly but not dramatically affected by the seasonal variations. The intensity of the Rayleigh molecular scattering as well as of the molecular oxygen line absorption show only very tiny variations. There is expectedly no scaling factor for oxygen (nor is there any for nitrogen) since the column abundance of the dominant constituents is basically driven by the pressure temperature equilibrium.

2.1.2 Scaling factors for water and ozone

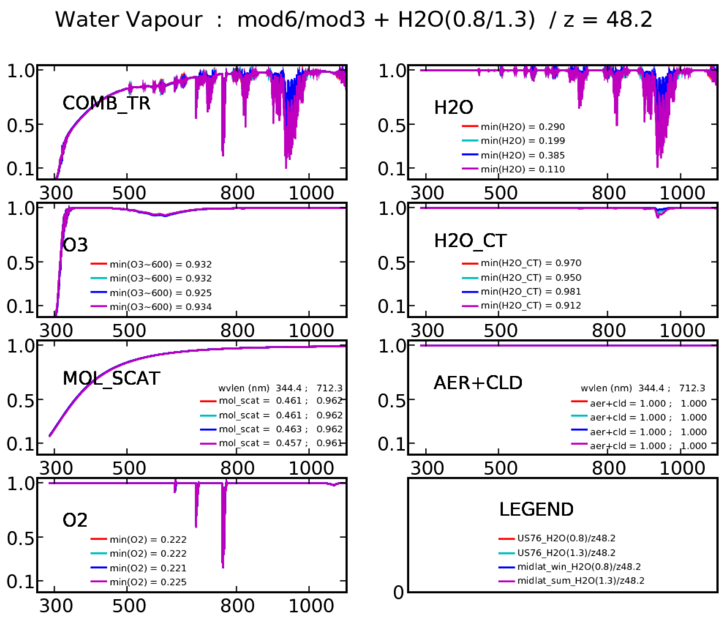


Figure 2.1.2 Same as 2.1.1 Water vapour variations with respect to season average are forced via the Modtran H2O scaling factor.

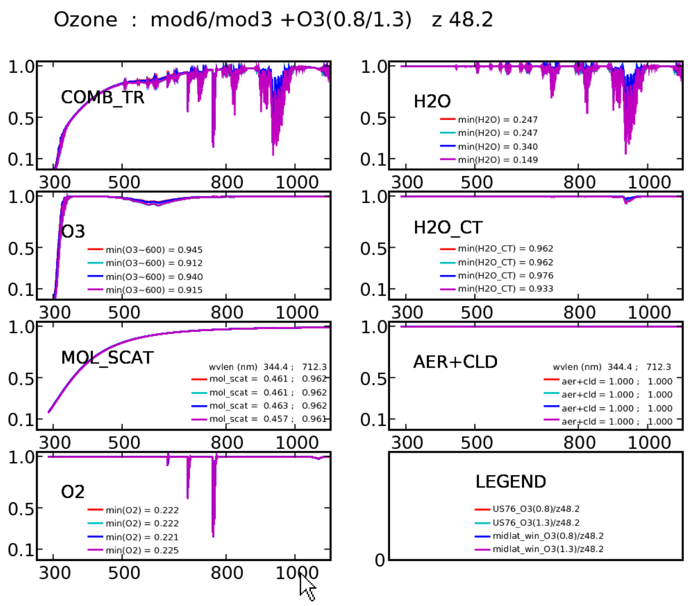


Figure 2.1.3 Same as 2.1.1 Ozone vapour variations with respect to season average are forced via the Modtran O3 scaling factor.

2.1.3 Cirrus Clouds

Astronomical observations are only concerned by thin cloud layers which would leave a few photons reach the telescope. Modtran has two standard cirrus models which can play this role. They are implemented by setting parameter ICLOUD to 18 (moderate cirrus) or 19 (subvisual).

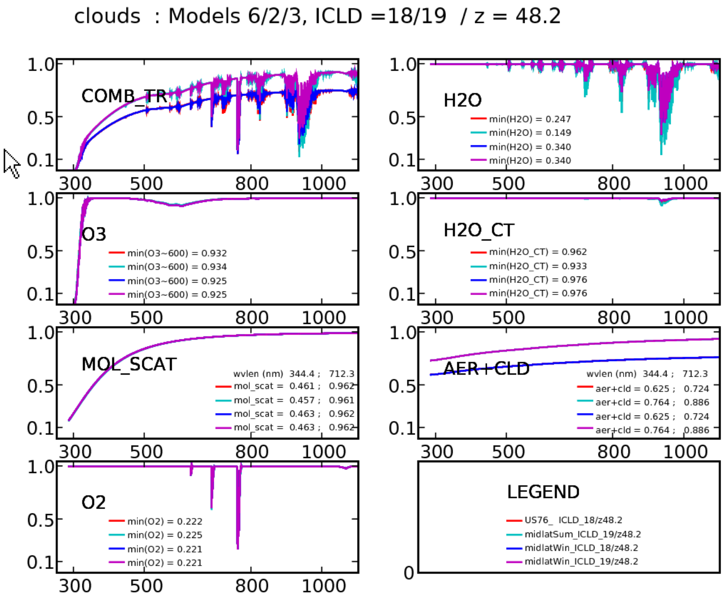


Figure 2.1.4 Same as 2.1.1 Cirrus clouds are forced into the picture

Being made of water droplets or fine ice particles, these clouds generate Mie diffusion, so, their spectral impact is not basically different from aerosols. For this reason only one kind of cirrus has been implemented in the scenarios.

2.1.3 Airmass versus zenith distance.

Airmass is not a straightforward function of the zenith distance. There are a number of numerical approximations published in the literature, involving a more or less detailed and realistic description of the local atmosphere in its relation with gravity and altitude. Modtran has its own way of doing so, simply by integrating the total pressure along each slant path so it takes into account both local gravity and altitude.

. The MODTRAN model of airmass versus zenith angle is suitably approximated by :

$$\varsigma = \frac{1}{\cos(z)} \; ; \; \chi = \log(\varsigma) \qquad (2.1)$$

$$X(z) = 1.00003873 \; \sigma \; -0.00548117 \; \chi^2 \; + 0.00832316 \; \chi^3 \; -0.00711221 \; \chi^4 - 0.00003873$$

This approximation fits the Modtran slant path numerical integration to better than 10^{-4} rms whatever the model and up to zenith angle 75.5 degrees. It is valid only for the altitude and latitude of the LSST Cerro Pachon site.

It is implemented both ways in two functions the Astrotools.py package associated with this simulation namely mdtram (*z_angle*) and mdtram2za (*airmass*) :

The trend of residuals of this fit versus airmass is shown in figure 2.1.5, in four frames corresponding to growing degrees of the fit approximation. The figure shows that the fourth degree approximation is needed to avoid small systematics.

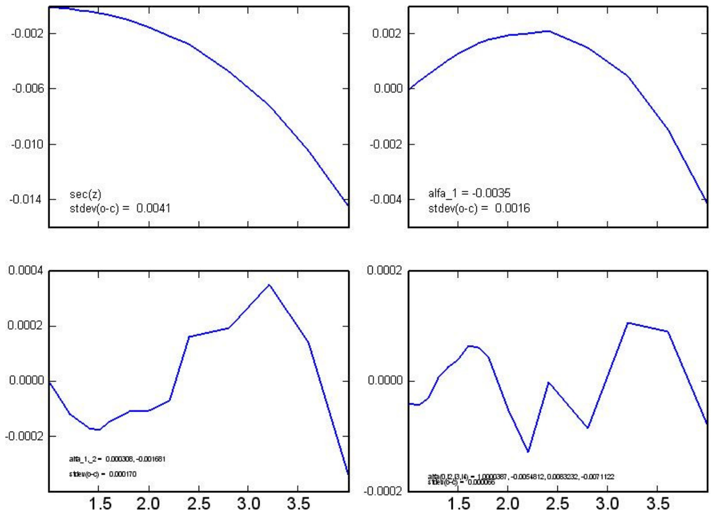


Figure 2 1.5 polynomial approximation of Modtran airmass: Trend of deviation of this fit with airmass at various approximations,

2.2 Water vapour control

Irrespective of the vertical structure of the model, the spectrum of water absorption is entirely determined by the total water vapour column above the observer. However there is not one single parameter to control this quantity in the Modtran parameter set. **The continuous water driving parameter in Modtran is the amount of water vapour relative to some seasonal reference value.** There is no way to cover the whole range of possible cases with this single parameter operating on only one seasonal model : Depending on the season, the vertical temperature structure of the atmospheres determines thresholds where the relative humidity reaches saturation once this is reached, Modtran blocks the water vapour density[4]. In our meteorological scenarios we first fix the time dependence of the vertical absolute water vapour column, then introduce a season and model dependent corrective factor to convert this quantity into relative.

2.2.1 from Modtran model and season dependent h2o drivers to absolute water vapour column

A series of test Modtran runs did check that the water spectrum is controlled by one single atmospheric quantity which is the water vapour column above the observer. However the temperature and pressure structure of the atmosphere does influence indirectly via

1. The water vapour saturation which is temperature dependent, thus allowing less water vapour in cold air. In the real atmosphere, once saturation is reached, water in excess condensates into fogs or clouds. Modtran computations fix the water vapour absorption at the saturation limit. The effect of fogs and clouds has to be forced by introducing aerosols or clouds. In the *MakeAtmos.py* routines which generates the lists of parameters spectra, we generate aerosols randomly subject to the condition that the water vapour approaches the season dependent saturation limit. Under US76 temperature conditions, water saturation happens by h2Ofact = 2 (water column 2.8) . Under mid lat winter conditions, this limit comes as low as h2Ofact =2 (water column 0.60):

2. The vertical distribution of water vapour in the column. Simply because when pressure is high, gases concentrate in the lower layers. Then, while in Modtran the total water column above sea level is simply a season and model dependent constant multiplied by a time dependent water factor, the growth curves of water extinction obtained are discontinuous at each season/model change if plotted against the total vertical column of water which is given by Modtran outputs above the sea level. To restore continuity we had to correct the

[4] The extra quantity of water vapour is not converted to water droplets or anything else, it is just lost while the aerosols are introduced separately by their own drivers.

water factor by another factor which is obtained as the fraction of the water column above the altitude of the LSST.
The ratio h2ofact(>LSST)/h2ofact(>sealevel) for model US76 being used as reference, it is modified by 0.98 for mid_latitude winter and 1.17 for mid latitude summer.

relat H2O col A	mod/seas B	season h2o col C (altitude scaled)	Modtran h2o factor A/C	absolute h2o col (atm.cm)
0,200	3_winter	0,8534	0,234	89,85
0,400	3_winter	0,8534	0,469	179,69
0,600	3_winter	0,8534	0,703	269,54
0,800	3_winter	0,8534	0,937	359,38
1,000	3_winter	0,8534	1,172	449,23
1,200	6-US76	1,4164	0,847	539,07
1,400	6-US76	1,4164	0,988	628,92
1,600	6-US76	1,4164	1,130	718,76
1,800	6-US76	1,4164	1,271	808,61
2,000	2-summer	2,5396	0,788	898,45
2,200	2-summer	2,5396	0,866	988,30
2,400	2-summer	2,5396	0,945	1078,14
2,600	2-summer	2,5396	1,024	1167,99
2,800	2-summer	2,5396	1,103	1257,83
3,000	2-summer	2,5396	1,181	1347,68
3,200	2-summer	2,5396	1,260	1437,52
3,400	2-summer	2,5396	1,339	1527,37
3,600	2-summer	2,5396	1,418	1617,21

Table 2.2.1 Gives in column A /C the scaling factor to be entered in MODTRAN depending on the season to reach the absolute water vapour column indicated in the last column.

This table is established at zenith, at larger airmass it was just checked that the water vapour column follows the airmass (see 2.1.4 for a numerical approximation of the airmass consistent with the Modtran atmosphere).

Given a set of Modtran model parameter it is thus obvious to get the total amount of water vapour along the line of sight as :

$$\omega = h2o\_fact \times season\_fact(mdl) \times X(z) \qquad (2.2)$$

In this equation,

- *h2o_fact* is the water vapour factor entered in Modtran cards,
- *season_fact(mdl)* is a season/model dependent factor (column C in above table)
- *X(z)* is the airmass as from equation (2.1).

Actually the normalization factor to the Modtran total column H2O for the line-of-sight path in Atmos x cm is 449.23 :

$$Col(h2o) = 449.23\,\omega \qquad (2.3)$$

2.2 Growth curves of water vapour spectral lines

The idea had been raised that the whole complexity of the Modtran mechanisms could be short circuited for our needs, by identifying a few absorption contributors (water vapour, ozone, …), each one driven by one single parameter related to the amount of the contributor in the column. The transmission spectrum of these components being obtained from a single pattern established at a reference amount an d scaled to the actual amount in the column.
This cannot be achieved so simply, due to the complexity of the spectral behaviour, the water spectrum is the most complex case. For one thing, due to the temperature dependant water vapour saturation limit, the number of water vapour molecules along the light path does not grow linearly, neither with the airmass, not with the ground humidity. For the other thing, due to optical saturation of narrow lines, the spectral pattern change is complex yet quite predictable.

We have established from a series of Modtran runs, and for each combination of season and model parameter, wavelength dependent growth curves as a function of the actual water vapour column as it is parameterized.

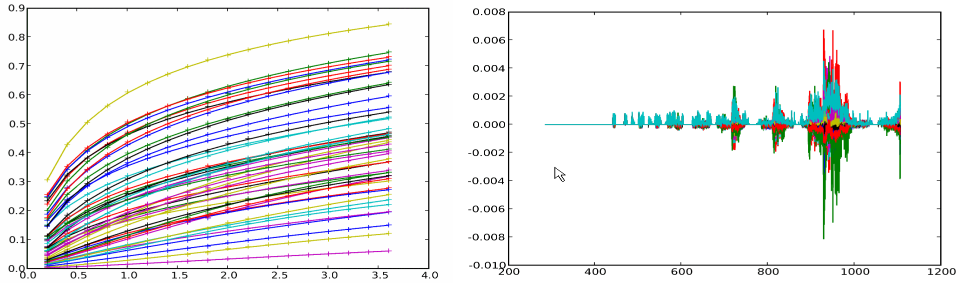


Figure 2.2.1: Fraction of light absorbed versus column of water vapour in 50 wavelength bins between 926.8 and 948.8 nm .Plus marks are the results of the Modtran radiation transfer computation along the slant path. Continuous lines show the adopted polynomial approximation (left). Residuals of polynomial approximation at all wavelengths (right).

2.3 ozone control

A series of experiments was performed to check that the total column absorber amount along the line of sight is the only effective driver of ozone absorption. Just as in the case of water vapour, this is established by varying arbitrarily the parameters (season model, O3 scaling factor, air mass), then getting from the Modtran outputs the calculated total O3 column along the line of sight and the Modtran calculated **ozone** transmission at 4 selected wavelengths.

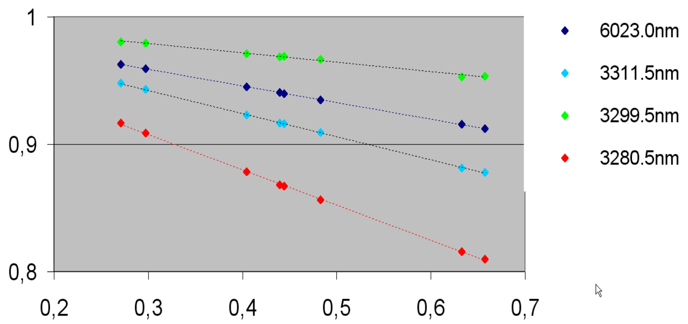
- One at the minimum of the shallow ozone transmission deep λ = 6023.
- The other three are at the top of two narrow absorption lines in the UV and at the bottom between them. In the region where there is a strong gradient of the continuum.

We plot transmission versus ozone column in figure 2.3.1. the dependence at the three wavelengths is remarkable over a wide range of the ozone column. Departures from linearity are order of a few 10^{-4}, approaching 10^{-3} only in the complex combination of lines and continuum gradient in the UV.

Table 2.3.1 Transmission at four typical wavelengths versus O3 column

Mod/ fact / airmass	Col O3 ***Atm.cm***	**O3 Trans 6023.0 *nm***	**O3 Trans 3311.5 *nm***	**O3 Trans 3299.5 *nm***	**O3 Trans 3280.5 *nm***
6/ 0.8/ 1.0	0,2706	0,9629	0,9478	0,9806	0,9168
3/ 0.8/ 1.0	0,2972	0,9594	0,9431	0,9794	0,9090
6/ 0.8/ 1.5	0,4045	0,9452	0,9230	0,9711	0,8782
6/ 1.3/ 1.0	0,4397	0,9405	0,9166	0,9687	0,8683
3/ 0.8/ 1.5	0,4444	0,9398	0,9161	0,9693	0,8671
3/ 1.3/ 1.0	0,4830	0,9348	0,9091	0,9667	0,8564
2/ 1.3/ 1.5	0,6329	0,9155	0,8813	0,9530	0,8156
6/ 1.3/ 1.5	0,6572	0,9124	0,8779	0,9535	0,8097
	rms dev	**0.0002**	**0.0003**	**0.0009**	**0.0007**

Figure 2.3.1 : transmission versus total column ozone at four typical wavelengths



2.4 oxygen control

Not implemented (03/2010)

2.5 aerosols control

2.5.1 Simulation versus calibration approach

a) Calibration model for aerosols

In the calibration approach developed by David Burke to extract the atmosphere transmission spectrum from ground based stellar photometry, the aerosol wavelength dependent optical depth[5] is modelled by a single power law:

$$\tau(z,a,t,\lambda) = (\tau_0 + \tau_1 t + \tau_2 . \tan(ha)) \left(\frac{\lambda}{\lambda_{ref}}\right)^{\alpha}$$
$$transmission = \frac{Iground}{I_0} = e^{-\tau} \tag{2.4}$$

here I_0 is the intensity out of atmosphere and λ_{ref} =675 nm. So there are only three optical depth unknown terms plus one single power parameter to fix the wavelength dependence.

b) Modtran aerosol spectrum

On the contrary, Modtran does not assume a law for the optical depth. Optical depth at each wavelength is derived from an assumed description of the aerosol particle properties and their vertical distribution. Then the spectrum is the result of a radiation transport calculation. Figure 2.5.1 shows the resulting spectra for a two series of Modtran parameter sets (see below for the meaning of these parameters), while Figure 2.5.2 reports the results of various attempts to approximate these spectra via either a third degrees polynomial fit or a power law fit.

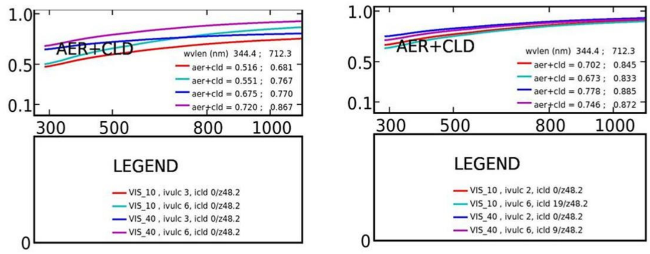


Figure 2.5.1 spectral transmission of aerosols under various Modtran parameterizations

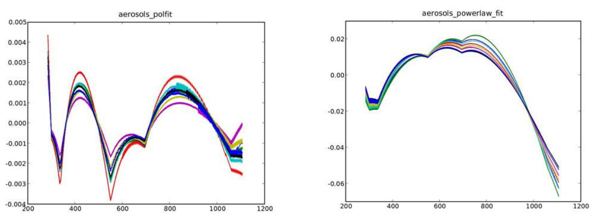


Figure 2.5.2

Obviously the two degrees of freedom of the power law fit does not offer a sufficient flexibility to represent the absorption by the complex blend of aerosol particles, resulting in systematic deviations beyond 0.02. With 4 degrees of

[5] The fraction of light making through the atmosphere depends of the three factors : size (s), density(ρ), opacity (κ) of absorbing particles, which can be condensed into a single value τ the ***optical depth***. Mathematically,

$$\frac{I}{I_0} = e^{-\kappa\rho s} \qquad \frac{I}{I_0} = e^{-\kappa\rho s}$$
$$= e^{-\tau} \qquad = e^{-\tau}$$

Mis en forme : Police :8 pt

freedom, the polynomial fit offers a more flexible approximation, and residuals below 0.002. The four cusps simply reflects the fact that Modtran evaluates rigorously the transmission at only four wavelengths in the domain of interest here (plus neighbouring points in the infrared and ultraviolet and interpolates). Details about these Modtran features can be found in the Modtran Mod4V3R1 user manual in the legend of table 10. The useful feedback of these attempts is that modtran aerosols do not rely upon simplifying assumptions that would unduly ease the calibration task.

c) Modtran aerosol parameters

There are four layers of aerosols each defined by its altitude and vertical extent, different types of particles (involving various particle size distributions) and adjustable column density. It is essential for the validation of the calibration scheme through simulations that the Modtran approach by integration of the physical components be maintained.

The default Modtran aerosol parameterization involves :

- ZAER11 and ZAER12 which are the lower and upper altitude of the bottom aerosol layer
- ZAER21 and ZAER22 which are the lower and upper altitude of the bottom aerosol layer

Default layer bottoms are fixed to 1 and 2 km respectively, tops to 3 and 11 km.

- VIS which is the ground visibility (in kms) determining the density of the ground aerosol layer at ground level.
- IVULC which is the driver of the volcanic aerosol (see Table 1 below), only options 0,2 and 5 have been used being made of dust the volcanic aerosol contribution is mainly to modify the spectal index of the Mie diffusion
- ISEASON which governs the seasonal dependence of the aerosol structure
- ICLOUD driving the presence of sub visual cirrus (ICLD=19) . Or absence (ICLD=0)

Table 2.5.1.

IVULC Corresponding to the Different Choices of Extinction Coefficient Model and the Vertical Distribution Profile(from MODTRAN Manual).

<table>
<tr><td rowspan="5">EXTINCTION MODEL</td><td rowspan="2"></td><td colspan="4">VERTICAL DISTRIBUTION</td></tr>
<tr><td>BACKGROUND STRATOSPHERIC</td><td>MODERATE VOLCANIC</td><td>HIGH VOLCANIC</td><td>EXTREME VOLCANIC</td></tr>
<tr><td>BACKGROUND STRATOSPHERIC</td><td>0,1</td><td>6</td><td>7</td><td>-</td></tr>
<tr><td>AGED VOLCANIC</td><td>-</td><td>2</td><td>4</td><td>-</td></tr>
<tr><td>FRESH VOLCANIC</td><td>-</td><td>5</td><td>3</td><td>8</td></tr>
</table>

2.5.2 Generating local aerosol anisotropy

Atmosphere anisotropies will be generated as variations of the parameters driving aerosol extinction expressed as functions of horizontal coordinates. Thus given a LSST pointing defined by Ra-Dec and time, azimuth and zenith angle should be derived to interrogate the atmosphere file and generate the sequence file entry from which the Modtran spectrum is generated.

Each azimuth dependent aerosol parameter must be designed to secure continuity across the zenith.
The most convenient driver of standard aerosols (mist) and light fogs is the ground visibility parameter σ (the Modtran parameter VIS in kilometres). Azimuth dependence can be implemented quite simply by a sine oscillation of σ between $(\sigma_0 - \sigma_1)$ and $(\sigma_0 + \sigma_1)$:

$$\sigma(a) = \sigma_0 + \sigma_1 \sin(a - a_0) \tag{2.5}$$

However this would result in a discontinuity at the zenith. In order to force continuity, the sine term must be weighted by a factor $\sin z$:

$$\sigma(a) = \sigma_0 + \sigma_1 \sin(a - a_0) \sin z \tag{2.6}$$

This would however over smooth the modulation at large air masses. A more sensible approach might be given by equations(2.7). In this formulation the smoothing factor operates only at small airmass (airmass > 1.4).

$$
\begin{cases} \sigma(a) = \sigma_0 + \sigma_1 \sin(a - a_0) \quad , \quad z > \dfrac{\pi}{4} \\ \sigma(a) = \sigma_0 + \sigma_1 \sin(a - a_0) \sin 2z \, , \; 0 \le z \le \dfrac{\pi}{4} \end{cases} \tag{2.7}
$$

This is implemented in the ***Makesequence_4.py*** module.

2.5.3 Approximation for transmission at 675 nm

The collaboration requested a separate indicator of the amount of aerosols involved, by convention, it was agreed that the aerosol optical depth (or transmission) at 675 nm would play this role. Modtran4 in its .tp7 output file gives separately the transmission spectrum of each one of the main components, including the aerosols, however this output uses prohibitive amounts of disc space when it comes to producing hundredth of thousands of spectra per year of LSST simulations. It was thus searched for an approximation which could be deduced from the Modtran input parameters without replaying the full atmosphere calculation.

A series of models were computed for all the combinations of model parameters used in each simulation, each combination being computed for a set of 9 values of the Modtran continuous aerosol driver VIS and a set of 5 increasing zenith distance, thus producing a mesh of values of τ_{675} covering the whole useful (VIS,Z) space.

Then a polynomial approximation is fitted by least squares over this mesh. The approximation is to is good to better than $3x10^{-4}$ in transmission across the whole useful space.

The module which computes and plots the 2D polynomial approximation from a series of experiments is ***aerosol_T675_2D_multi2.py*** it stores the coefficients in a file with suffix ***…_t675_fitresults.txt*** there is a prefix identifying the relevant set of experiments. And the directory is the generic directory for the set of experiments (namely ***T04.results*** for Opsim129.01, ***T05.00*** for Opsim129.02).

The coefficients are retrieved and used by the module ***shape_store_spectra_[#].py*** (***#***=8 on Decembre 15 2009) at the end of a long simulation. For each spectrum identified by its rank in the series of LSST pointings the set of four Modtran parameters which caracterize the aerosol type (Model, Iseason, Ivulc, Icld) are first retrieved from the associated *…_parmlist.dat* file, together with the LSST pointing identifier, time, Zenith distance and VIS. Eventually the spectra are stored column wise with three lines of headers on top of each spectrum the third line is τ_{675} or T_{675} depending on versions.

2.5.4 Aerosols in meteorological scenario *meteo.01* : Heavy rural

The first long term atmosphere simulations were intended to check the robustness of the calibration approach based on observing reference stars at a spectroscopic auxiliary telescope operating night long. So, simulated atmospheres had to challenge the calibration procedure by introducing irregular (yet physically realistic) atmosphere variations inducing strong transmission irregularities. Aerosols are one of the most challenging unknowns of this problem. Starting with the default structure of aerosol layers, and the limited options of this default scenario, it soon appeared that reaching high levels of aerosol extinction at the altitude of the LSST that could be modulated via the ground visibility parameter requested a "rural" regime. This is not a normal situation on a selected mountain site, but it was appropriate as a bench for the calibration procedure. This rural regime combined with the "azimuth anisotropy" described in section 2.5.2. it offers all the desired difficulties to the calibration. The whole scenario ***meteo.01***, which was combined with the first three year of LSST observation history Opsim129 to produce the series of spectra, Opsim129.01 is described in section 3.1. We describe here its aerosol component.

a) Modtran parameters

In simulation ***meteo.01***, the following parameterization of aerosol is used

Ground aerosol layer characteristics

- **ihaze = 1** # aerosol driver **IHAZE** set to 1= rural (other possible values are : 0 = none; 6 = Tropospheric)
- **ZAER11 = 1 ; ZAER21 = 4.** : Low aerosol layer between 1 and 4 km meaning a rather heavy aerosol layer.
- **ZAER12 = 2 ; ZAER22 = 11.** : Tropospheric aerosol layer from 2 to 11 km.
- **SCALE1** and **SCALE2** are set to 1. (i.e. no scaling)
- Season names = ['Summer', 'Fall', 'Winter', 'Spring'] # Southern hemisphere
- Season model = [2,6,3,6] modtran seasonal models
- Aerosol season = [1 , 2, 2, 1] ISEASON = 1 (summer, spring) or 2 (fall, winter)

- There is also a significant influence of the season dependent atmosphere structure model so Model is either 6 (US76, on spring and fall) or 2 (Mid latitude summer) or 3 (Mid l winter)

So the active combinations of **MODEL** and **ISEASON** are:

- Summer (2,1)
- Fall (6,2)
- Winter (3,2)
- Spring (6,1)

Volcanic aerosol types

Parameter Iv in table 2.5.3 is the Modtran IVULC, governing the volcanic aerosols. it is 0, 2 or 5 according to the definitions given in table 2 .5.1 above. In scenario meteo1 only 2 and 5 are actually used.

Cloud types

Cloud driver (**ICLOUD** for modtran) is either 0 (no cloud) or 19 (subvisual cirrus)

Time variation drivers : See 3.2.2

b) Approximation for 675nm optical depth

According to the approach described in § 2.5.3, in order to get a predictable measure of the Modtran aerosol extinction response to the adopted set of models and parameters, a 2D-third order polynomial was least-square fitted to the variation of τ_{675} versus VIS and Airmass under the complete series of Modtran parameter sets used in the scenario..

This is summarized in Table 2.5.3 below where coefficient α_{ij} means order i in x and order j in y , x is VIS and y is airmass.

$$\begin{aligned} &T(x,y) = \alpha_{00} + \alpha_{10}x + \alpha_{01}y + \alpha_{20}x^2 + \alpha_{02}y^2 + \alpha_{11}xy + \alpha_{30}x^3 + \alpha_{03}y^3 + \alpha_{21}x^2y + \alpha_{12}xy^2 \\ &x = VIS,\ y = airmass\ \ ,T = transmission\ ,\ \tau = optical\ depth \\ &T = e^{-\tau} \end{aligned} \tag{2.8}$$

Table2.5.3 : Aerosol τ_{675} approximation : Coefficients for scenario ***meteo .01***
See equations (2.8) for the signification of coefficients

	Md,Is,Iv,Ic	α_{00}	α_{10}	α_{01}	α_{20}	α_{02}	α_{11}	α_{30}	α_{03}	α_{21}	α_{12}	σ
		x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}
53	6,1,0,0	9279480	48526	-1944732	-1048	87768	36541	7	-1660	-260	-1035	2884
54	2,1,0,0	9279862	48540	-1946357	-1048	88592	36555	7	-1807	-260	-1035	2881
55	3,1,0,0	9292137	47339	-1939488	-1016	86364	36421	7	-1570	-259	-1019	2842
56	6,2,0,0	9347521	45024	-1728939	-1001	63401	35807	7	-1249	-265	-784	2578
57	6,1,2,0	9262145	49066	-2092201	-1044	113819	34570	7	-2602	-240	-1170	2792
58	6,1,5,0	9251079	49423	-2120950	-1042	119975	33831	7	-2877	-233	-1186	2759
59	6,1,0,19	9263518	48601	-2041306	-1034	101518	34917	7	-1552	-243	-1134	2795
60	6,1,2,19	9243292	49437	-2189960	-1036	130390	32916	7	-2761	-223	-1261	2715
61	6,1,5,19	9257815	48129	-2225777	-1002	136450	32615	7	-2859	-220	-1300	2671
62	6,2,2,0	9334605	44923	-1866570	-973	85199	33717	7	-1863	-243	-913	2608
63	6,2,5,0	9339688	44409	-1901535	-958	89963	33354	7	-1708	-238	-971	2554
64	6,2,0,19	9336248	44827	-1832282	-973	78858	34090	7	-1487	-246	-899	2663
65	6,2,2,19	9308795	45720	-1964742	-976	98054	32189	7	-1529	-226	-1023	2519
66	6,2,5,19	9321328	45056	-2010415	-958	108382	31886	7	-2246	-222	-1077	2576
67	3,2,0,0	9356028	44370	-1730380	-981	65300	35718	7	-1658	-265	-769	2620
68	3,2,2,0	9334567	45051	-1867794	-977	85955	33698	7	-1915	-242	-922	2556
69	3,2,5,0	9334930	44810	-1901625	-967	91281	33235	7	-1961	-237	-967	2558
70	3,2,0,19	9339476	44744	-1834863	-974	78695	34216	7	-1359	-247	-914	2528
71	3,2,2,19	9332685	43974	-1966320	-934	97834	32277	6	-1414	-227	-1038	2559
72	3,2,5,19	9318274	45362	-2010752	-967	108538	31887	7	-2352	-223	-1068	2503

2.5.5 Aerosols in meteorological scenario *meteo.02* : Mauna Loa like.

The second step of the aerosol simulations was to produce a more realistic scenario offering not only a broad variety of aerosol conditions, but also a more realistic sample of the conditions likely to prevail on the LSST site. This step was requested by the collaboration earlier than initially planned. Reference data were taken from the AERONET aerosol optical depths obtained at the Mauna Loa (Hawaii) site, as reported in Stubbs et al. (2007)[6]. Figures 2.5.1 and 2.5.2 are reproduced from this paper.

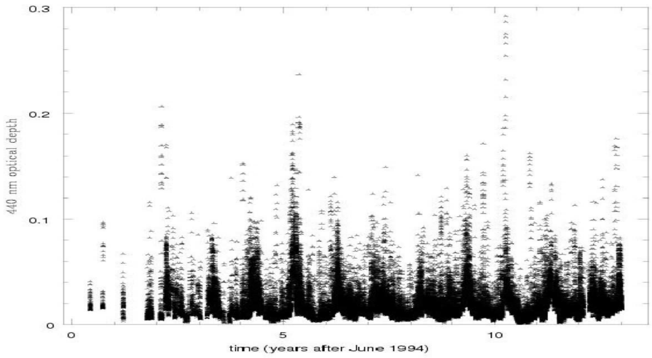


Fig. 2.5.1 . Aerosol Optical Depth. The graph shows the daytime aerosol optical depth at 440 nm over time as reported from solar flux measurements by the AERONET system on Mauna Loa, near the site of the PanSTARRS-1 system. The vertical axis is optical depth τ where a fraction $e^{-\tau}$ is transmitted through one airmass. Time is in years after June 1994). There is clear evidence for seasonal cycles, as well as considerable variation on short timescales.

The 440 nm measurements are plotted in figure 2.5.1 over 13 years, while figure 2.5.2 shows measurements at 4 wavelengths (including our 675nm reference) over a shorter 72 days period. Comparing these plots with the reference panel of figure 3.1.1 below, shows (unsurprisingly) that the rural scenario is not appropriate the high altitude situation:

- The baseline 675nm aerosol optical depth is too high by at least a factor 5
- Long time scale seasonal oscillation has almost the appropriate amplitude
- Short time scale excursions to large amplitudes are on the contrary underestimated

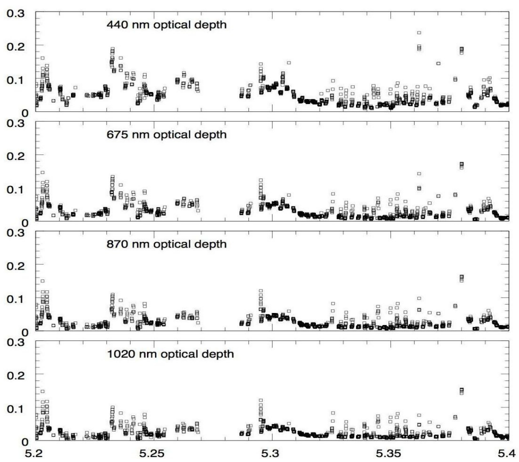


Figure 2.5.2 : Mauna Loa aerosol optical depths at 4 different wavelengths over 72 days.

[6] Stubbs et al. 2007, arXiv:0708.1364v1 [astro-ph] 10 Aug 2007 *"Towards More Precise Survey Photometry for PanSTARRS and LSST: Measuring Directly the Optical Transmission Spectrum of the Atmosphere"*

In the observed Hawaii series, the τ_{675} indicator oscillates between 0.01 and 0.05 over monthly timescales, inside these periods, there are shorter random peaks of high absorption ceiling by 0.20 or so. We roughly mimic this behaviour with a seasonal oscillation of 0.04 +- 0.03, corrected by long segments down (typical time scales 20 days, amplitude reduced by factor 0.5) and short segments up (typical time scales 7 days, amplitude raised up to τ_{675}=0.20.

a) *Modtran parameters*

Ground aerosol layer characteristics

- **ihaze = 1** # aerosol driver **IHAZE** set to 1= rural (other possible values are : 0 = none; 6 = Tropospheric)
- **ZAER11 = 1 ; ZAER21 = 3.** : Low aerosol layer between 1 and 4 km meaning a rather heavy aerosol layer.
- **ZAER12 = 1 ; ZAER22 = 3.** : Tropospheric aerosol layer from 2 to 11 km.
- **SCALE1 is tuned to the adopted VIS according to equation** (2.9) in order to produce the desired optical thickness.
- **SCALE2** is set to 1. (i.e. no scaling)
- **Other parameters** remain unchanged with respect to *meteo01*.

Volcanic aerosol types

- **IVULC**, is 0, or 2 (none or moderate old) according to the definitions given in table 2.5.1 above.

Time variation drivers :

- See 3.3.2

More about tuning VIS and SCALE for more realistic hazy aerosols

On trying to obtain the appropriate τ_{675} statistics, standard parameterizations of MODTRAN for water droplets aerosol layers as used in ***meteo.01*** (Rural or tropospheric), does not offer the required flexibility. Playing with authorized extreme values of the ground visibility parameter (VIS) would typically produce τ_{675} variations in the range 0.07 through 0.30 far above any expectation in a good astronomical mountain site. There is no way in the standard schemes to get below this value because the MODTRAN SCALE parameter has only scale up options, while the VIS parameter (ground visibility) influences only the lower aerosol layer. Scaling down is obtained by lowering the altitude of the top of the lower layer down to ZAER12 = 2 (km). Although this limit is set below the telescope altitude, there is still an effect and the modulation by and the VIS parameter is still active (strangely the "ground altitude" does not play this role). Setting ZAER12 to 1 km produces exactly the same result as 2 km, meaning that the effect at the telescope altitude is entirely driven by the upper layer of the troposphere. So, further sizing down the useful aerosol layer must be obtained by playing with layer 2 and above. In the following we keep the rural regime (IHAZE=1) rather than the tropospheric one (IHAZE=6) which introduces the additional difficulty that Modtran under this option deals with the lower and upper troposphere layers in combination as specified in the Modtran manual on page 31:

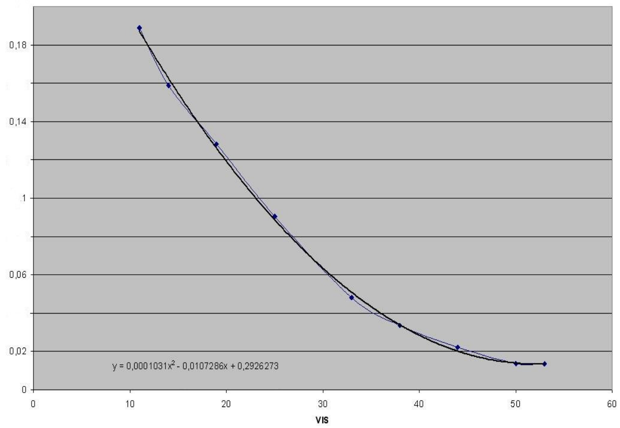
> *By this definition, the region of aerosol 1, for example, is from 0 to 3 km; the profile linearly decreases from a positive value at 2 km to zero at 3 km. Instead, in previous MODTRAN documentation this region is said to be from 0-2 km. In the MODTRAN upgrade, the ZAERi1 and ZAERi2 values refer to the bounding altitudes, which sandwich the entire region where the aerosol concentration is positive. Table 6 lists the default values of these bounding altitudes along with the commonly referred to region boundaries for each aerosol.*
>
> *One caveat with regard to the **CARD 2+** inputs should be noted. For the Tropospheric aerosol model (**IHAZE = 6**), MODTRAN combines the boundary layer (Aerosol 1) and tropospheric (Aerosol 2) regions; therefore, these region may not be scaled independently. Thus, the parameters used to scale the tropospheric aerosol model are min (ZAER11, ZAER21), max (ZAER12, ZAER22) and max (SCALE1, SCALE2).*

To reach the appropriate scales, it was necessary to get rid of the bulk of the high tropospheric layer by arbitrarily moving it below the altitude of the telescope. The lower layer which is sensitive to the VIS parameter was then scaled associating decreasing values of VIS (more aerosol density at ground level) with globally scaling up the low aerosol layer (using SCALE1). In practice, this is achieved with

$$\begin{aligned} &VIS(km) \in [11.0, 53.0] \\ &SCALE1 = \text{int}(-7.08\log(VIS) + 29.) \end{aligned} \tag{2.9}$$

This one to one correspondence allows to pilot the aerosol simulation with only one continuous parameter VIS While passing to MODTRAN the two parameters (VIS and SCALE1) it needs to explore the whole expected range of aerosol transmission. The resulting trend of the zenith τ_{675} (at the latitude and altitude of Cerro Pachon) as a function of VIS alone is plotted on the figure below. Equation (2.10) gives a convenient approximation to get the resulting zenith τ_{675} without running MODTRAN .

$$\tau_{675} = 0.0001031 vis^2 - 0.010729 vis + 0.2926 \qquad (2.10)$$



Mis en forme : Centré

Figure 2.5.3 : controlling optical thickness τ_{675} via the Modtran VIS and SCALE1 parameters via equation (2.9).

A sequence of typical τ_{675} aerosol optical depths covering 72 days taken out of the scenario ***meteo.02*** is plotted on figure 2.5.4 below, together with a comparable sequence taken from the Mauna Loa data, showing that the scenario mimics reasonably well the real data in terms of baseline value, amplitude and time scale of high depth excursions.

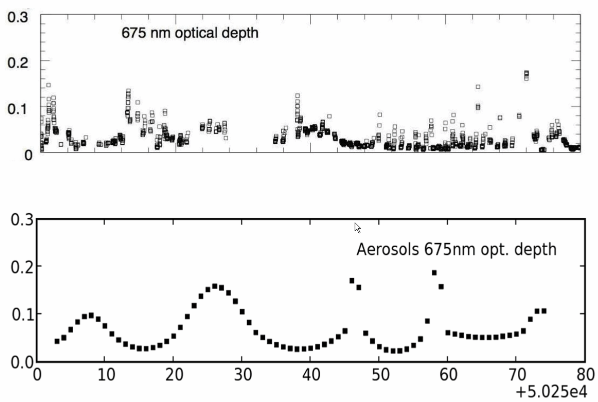


Figure 2.5.4 : Aerosol 675nm optical depth as observed at Mauna Loa Hawaii (top) over 72 days. Compared to a similar period extracted from the atmosphere scenario ***meteo.02***

b)Approximation for 675nm optical depth

Polynomial coefficients for the whole set of models used in simulation Meteo.02 are given in Table 2.5.4 below

Table2.5.4 : Aerosol τ_{675} approximation : Coefficients for scenario ***meteo .02***
See equations (2.8) for the use of coefficients

	Md,Is,Iv,Ic	α_{00}	α_{10}	α_{01}	α_{20}	α_{02}	α_{11}	α_{30}	α_{03}	α_{21}	α_{12}	σ
		x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}	x 10^{-7}
51	6, 1, 0, 0	9874525	-3523	-2422007	709	131127	70372	-12	-1526	-482	-2649	37210
52	(6, 2, 0, 0)	9870964	-3438	-2413043	708	128455	70385	-12	-1273	-483	-2624	37265
53	(2, 1, 0, 0)	9874671	-3543	-2421934	710	131170	70357	-12	-1507	-481	-2653	37225
54	(3, 2, 0, 0)	9872306	-3541	-2413966	709	128498	70433	-12	-1270	-483	-2628	37250
55	(6, 1, 2, 0)	9821650	322	-2547369	626	156434	66813	-11	-1578	-437	-3039	35619
56	(6, 2, 2, 0)	9824827	141	-2538368	631	155124	67012	-12	-1709	-440	-3003	35687
57	(2, 1, 2, 0)	9820479	384	-2545632	624	155467	66797	-11	-1416	-437	-3038	35649
58	(3, 2, 2, 0)	9826535	165	-2541930	628	156235	67080	-11	-1797	-440	-3018	35663
59	6, 1, 0, 19	9837630	-598	-2520783	647	152963	67677	-12	-2106	-448	-2951	36028
60	6, 2, 0, 19	9834952	-704	-2509342	648	147863	67814	-12	-1394	-449	-2940	36098
61	2, 1, 0, 19	9837810	-604	-2521224	647	153481	67662	-12	-2229	-448	-2944	35955
62	3, 2, 0, 19	9836649	-683	-2513207	648	149848	67803	-12	-1705	-449	-2948	35975
63	6, 1, 2, 19	9789073	3124	-2650789	565	181647	64237	-11	-2698	-406	-3296	34428
64	6, 2, 2, 19	9789262	2957	-2637584	569	178406	64421	-11	-2545	-408	-3262	34538
65	2, 1, 2, 19	9788963	3152	-2651209	564	182274	64206	-11	-2847	-406	-3290	34457
66	3, 2, 2, 19	9791405	2845	-2639576	572	178681	64463	-11	-2538	-408	-3271	34546

3. Meteo scenarios for long term simulations

We call ***meteo*** scenarios a list of heuristic rules describing the evolution of the main atmosphere components involved in the atmospheric extinction over long periods, including the algorithms required to translate these rules into Modtran parameters. The rules and the corresponding algorithms are structured by different time scales characterizing the typical variations of atmospheric phenomena.

3.1 Time scales

The longer timescale is season. Seasonality is obviously one of the major risks, since the same parts of the sky would be to some extent repeatedly observed through similar atmospheric conditions. In early versions, seasons are fixed : 3 calendar months from the 22nd of an equinox/solstice month to the 21rst of the next solstice/equinox. This rigid seasonality may lead to exaggerate the resulting systematics.

Seasons govern –

a) the vertical structure of the atmosphere (pressure, temperature) (currently via the choice of MODEL) which drives the amount of molecular oxygen and nitrogen (via pressure) thus influencing Rayleigh diffusion and oxygen molecular lines. It also drives (via temperature) the water vapour saturation point.
b) the amplitudes and typical timescales of molecular absorber variations (O3 and H2O)
c) the ranges and time scales of parameters governing aerosols
d) the frequency and duration of cloudy episodes.

The second longer timescales are order of magnitudes of say 10 days. It is the timescale over which the current meteorological situation evolves. These intermediate periods are called ***segments***. The segments are created as pseudo random exponential variates which scale lengths and associated amplitudes are specified for each season and each parameter (ozone segments, are independent of water vapour segments or aerosol segments)

Inside a segment, slowly varying parameters would either be constant or evolve following a sine curve added to the seasonal value with the associated random generated amplitude alternatively upwards and downwards. The phase of the sine is 0 at the start of the segment and π at the end. This is implemented by equations (3.1) giving the value of a parameter p as a function of time

$$
\begin{aligned}
&\overline{p}(t) = p_0 + p_1\left(\frac{2\pi}{365.}(t - t_0) + \phi_0\right) \\
&s(t) = s_0 + s_1\overline{p}(t) \\
&t_0 = MJD(mid\_winter) \\
&p(t) = \overline{p}(t) + \varepsilon(t)\,\gamma(t)\,s(t)\,\sin\left(\pi\frac{t - \tau(t)}{\delta(t)}\right)
\end{aligned}
\tag{3.1}
$$

Where

- t_0 is the MJD time of mid winter in the current year
- $\tau(t)$ is the start time of the current segment,
- $\delta(t)$ is the length of the current segment, it is generated as an exponential variates with scale δ_0
- $\gamma(t)$ is a random modulation of the amplitude. It is generated as a normal variate with unit mean and variance 0.5. In some cases, in order to care for physical realism or to avoid numerical singularities, it may be limited between a minimum γ_0 and a maximum γ_1 . $\gamma(t)$ is used to modulate the amplitude $s(t)$ of excursions above or below the current mean value $\overline{p}(t)$ of the considered parameter.
- $\varepsilon(t)$ is constant over one segment, it is alternatively +1 or -1 from one segment to the next it is in charge of implementing the old wisdom of weather experts : "*après la pluie le beau temps and vice versa*"

Scenarios are evaluated every other 0.01 day.

3.2 Meteo scenario .01 : a tour of effects generating significant variations

3.2.1 Parameters and atmosphere statistics

The permanent Modtran parameters of this scenario are given in ***§ 2.5.4.a);*** The time variation drivers governing equation (3.1) are given in table 3.2.1

Table 3.2.1 : Variability drives for scenario Meteo 1 (see § 3.1 for usage)

parameter	O3	H2O	VIS
(p_0 , p_1, ϕ_0)	$\left(1.05 , -0.35, -\frac{\pi}{2}\right)$	$\left(1.0 , 0.3, -\frac{\pi}{2}\right)$	$\left(40. , -10., -\frac{\pi}{2}\right)$
(s_0 , s_1)	$(0., 0.03)$	$(0.2, 0.)$	$(3.0, 0.)$
(γ_0 , γ_1)	$(0.1 , \infty)$	$(0.1 , \infty)$	$(0.1 , \infty)$
$\left(\delta_{0_{\text{Summer}}}, \delta_{0_{\text{Fall}}}, \delta_{0_{\text{Winter}}}, \delta_{0_{\text{Spring}}}\right)$	$(12,12,10,12)$	$(10,10,12,10)$	$(12,12,12,12)$

Cloud episodes (sub visual cirrus) surge with a probability of 2/10 when the water segment is up ($\varepsilon = +1$ in equation(3.1)) cloud episodes are short (0.5 days), but frequent.
There is a permanent yet moderate of old volcanic aerosol layer (IVULC=2) and an extra fresh layer (IVULC=5) in the middle of the third scenario year.

The resulting variations of the drivers for the main absorbers are plotted in figure 3.2.1 below over three years from January 1994 to January 1997. Concerning aerosols which are driven by several parameters, we give the resulting zenith optical depth of the aerosols. The scenario is by construction a caricature: Water is high in summer and low in winter (but the adopted amplitude is in no ways in relation with the temperature). Short timescale oscillations supposed to represent the surge of wet air masses are quite arbitrary. Same way the ozone is duly maximum in winter and minimum in summer, but the amplitudes of the oscillations is arbitrary. The more complex issue of aerosols is discussed in detail in section 2.5.5.

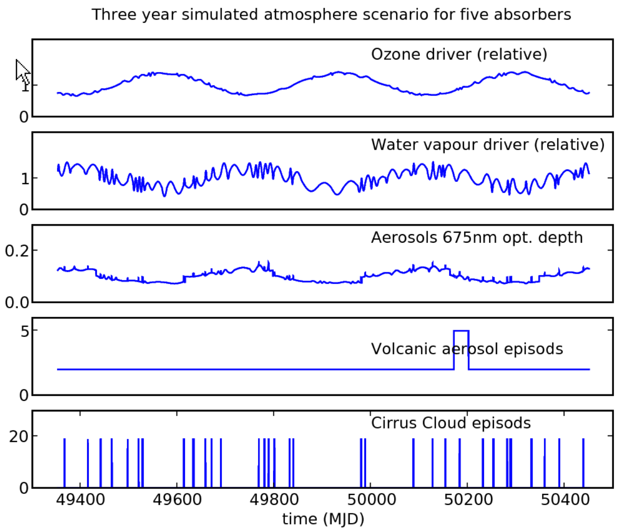


Fig. 3.2.1 : Atmosphere parameter history for simulation Opsim129.01

3.2.2 photometry statistics

The impact produced by the above described scenario of atmospheric fluctuations can now be evaluated in terms of LSST photometry.

For this purpose, we extracted from the three year Atmosphere history file meteo.01 described above the MODTRAN parameters associated to each LSST pointing as planned in the Opsim129 simulation, then tuned the MODTRAN inputs to each pointing (That is taking into account the field azimuth and zenith angle), then ran MODTRAN to get the transmission spectrum. Obtaining eventually transmission spectra for the atmosphere each of the about 10^6 LSST pointings along the 3 years of the scenario now labelled as Opsim129.01.

The statistics below are based on a sub sample obtained by picking 1 spectrum out of 300 resulting in 3804 spectra. Transmission spectra are convolved with the LSST filters instrumental transmission curves and integrated in each filter to calculate the magnitudes absorbed by the atmosphere in each filter. Actually what is obtained is magnitude deviations with respect to a reference spectrum[7] .

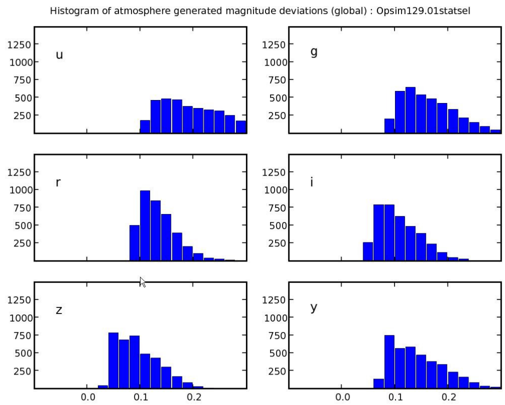


Figure 3.2.2 Histograms of atmosphere generated magnitude deviations for simulation Opsim129.01. The heavy tails of all histograms is generated by the adopted heavy rural aerosol scheme (see figure 3.3.2 for comparison)

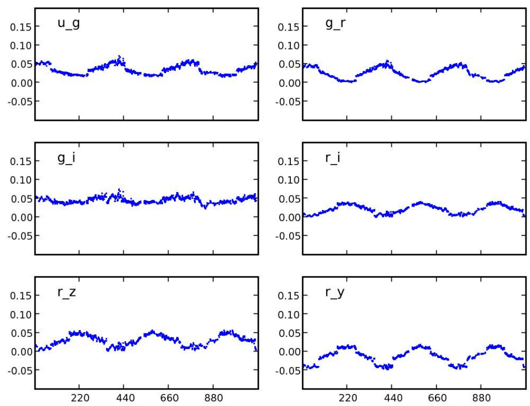


Figure 3.2.3 Trend of colour deviations with time in Opsim 129.01. The statistics is limited to small air masses (z < 30°). Clearly oscillations visible in u-g, g-r, r-i are phased with ozone and aerosols, redder indices reflect water and aerosols.

[7] In order to eliminate from the statistics very large effects simply due to obviously calculable airmass changes (which would hide the interesting variations), the absolute transmissions are not used, instead we use the ratio of the absolute transmission with that of one single reference atmosphere at the same airmass.

3.3 Meteo scenario .02 : 3 years with aerosols based on Mauna Loa statistics

3.3.1 parameterization and atmosphere statistics

The permanent Modtran parameters of this scenario are given in ***§ 2.5.5-a);*** The time variation drivers governing equation (3.1) are given in table 3.3.1

Table 3.3.1 : Variability drives for scenario Meteo 1 (see § 3.1 for usage)

parameter	O3	H2O	VIS
(p_0 , p_1, ϕ_0)	$\left(1.05 , -0.35, -\frac{\pi}{2}\right)$	$\left(1.0 , 0.3, -\frac{\pi}{2}\right)$	$\left(40. , +10., -\frac{\pi}{2}\right)$
(s_0 , s_1)	$(0., 0.03)$	$(0.2, 0.)$	$(8.5, 0.)$
(γ_0 , γ_1)	$(0.1 , \infty)$	$(0.1 , \infty)$	$(0.1 , \infty)$
$(\delta_{0_{Summer}}, \delta_{0_{Fall}}, \delta_{0_{Winter}}, \delta_{0_{Spring}})$	$(12,12,10,12)$	$(10,10,12,10)$	$(10,10,10,10)$
(VIS_{min}, VIS_{max})			$(11.,53.)$

Cloud episodes (sub visual cirrus) surge with a probability of 2/10 ; cloud episodes are short (0.5 days), but frequent. create 3 period of fresh volcanic aerosol with random durations (0,50 days)
There is no permanent volcanic aerosol layer (IVULC=0 by default); three periods have been placed randomly during these periods fresh volcanic aerosol (IVULC=5) with random durations (0,50 days) may surge.

The resulting variations of the drivers for the main absorbers are plotted in figure 3.3.1 below over three years from January 1994 to January 1997. The scenario is the same as meteo01 for and ozone. Aerosols
Follow now a statistics quite comparable to the Mauna Loa

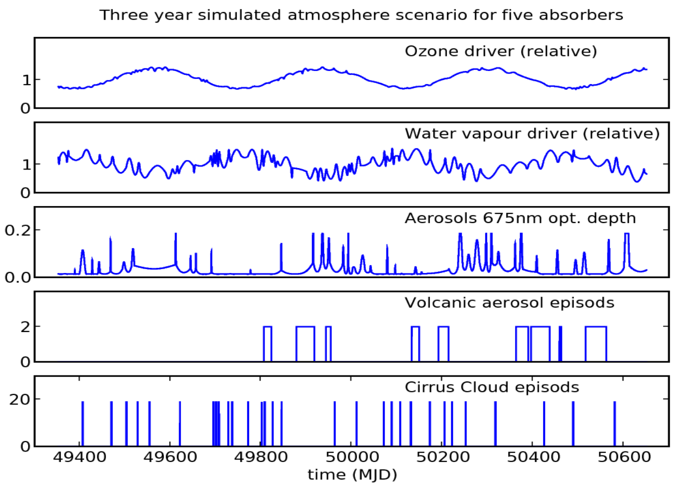


Fig. 3.2.1 : Atmospheric scenario for simulation Opsim129.02 the main differences with respect to figure 3.1.1 are the aerosol.

3.3.2 photometry statistics

The impact produced by the above described scenario of atmospheric fluctuations can now be evaluated in terms of LSST photometry. (See 3.2.2 for details)

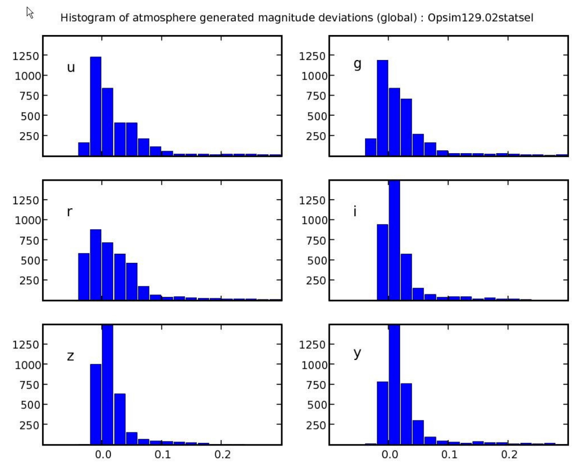


Figure 3.3.2 Histograms of atmosphere generated magnitude deviations for simulation Opsim 129.02

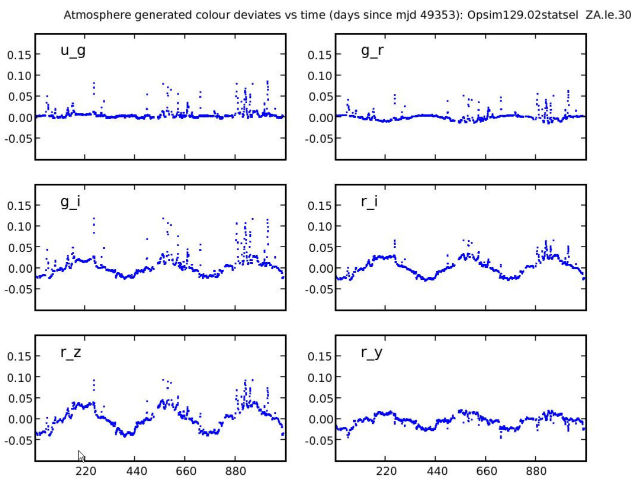


Figure 3.3.3 Trend of colour deviations with time in Opsim 129.02 In the absence of significant seasonal modulation of aerosols, the u-g colour shows no oscillation. The difference of behaviour between u-g and g-r suggests that information is available from LSST photometry alone to separate aerosol effects from ozone effects.

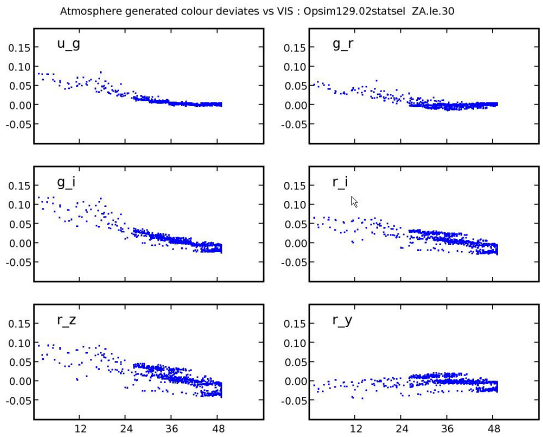


Figure 3.3.4 Trend of colour deviations with aerosol driver VIS in Opsim 129.02

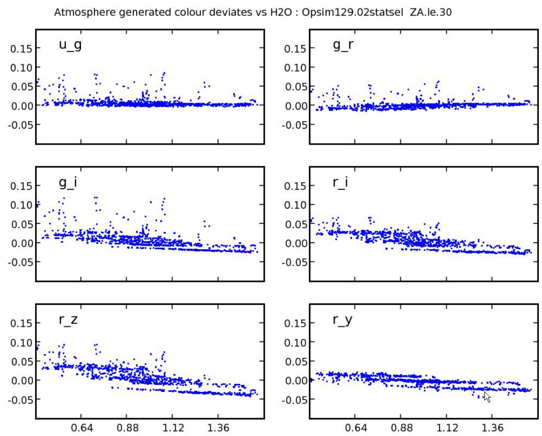


Figure 3.3.5 Trend of colour deviations with water vapour driver H2O in Opsim 129.02

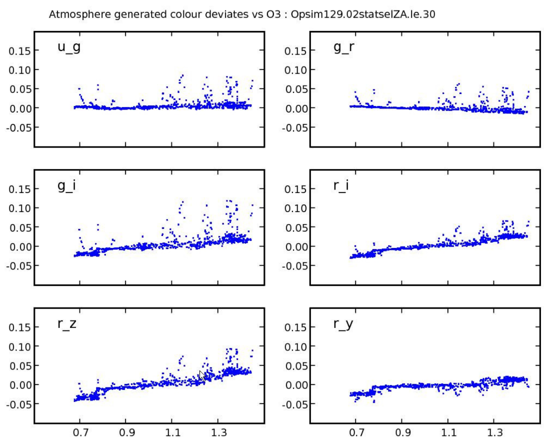


Figure 3.3.6 Trend of colour deviations with ozone driver O3 in Opsim 129.02

4. What next?

Toolbox portage

The next task, although not scientifically the most exciting, will be the transmission of this tool box to the collaboration. This includes standardizing the Python modules developed around the Modtran 4 kernel and documenting them, i.e. writing the second part of the current document: a technical user guide to the library of modules. There will be two steps.

The first step will be achieved within three months; it is limited to whatever is needed once an “Atmosphere History” file has been produced.

Transmitting the MakeAtmos.py module which includes all the meteorological science will be a more demanding task because it is a baroque machinery developed in the exploratory phase of this work as a patchwork and based on naïve algorithms. Whether it just needs some grooming or requires a more profound remodelling is an open question: if is to be used intensively by the collaboration for many simulations with many different scenarios, or if , even for less intensive use the naïve algorithms turn out to induce undesired effects, then only the later option is reasonable, otherwise

More on seasonality

Current long term atmospheric changes are essentially season based, the seasons are ruled by rigid calendar dates, this is likely to induce periodicities in the systematic effects. To some extent this systematics is desirable because if the calibration is not able to get rid of them, the effects will reflect in the mapping of cosmological phenomena. However if their systematisation is exaggerated it might induce an overestimation of the danger and impose to the calibration unnecessary complexities. Introducing some reasonable seasonal irregularities in future scenarios is not a major problem but it must be known that this is not the case currently (as obvious from figures 3.2.1 and 3.3.1)

Towards spectral self calibration

The photometry statistics presented in sections 3.2.2 and 3.3.2 demonstrate that the LSST photometry does contain significant signal on fluctuations of the atmosphere transmission spectrum. At this stage, it is reasonable to anticipate, but not yet demonstrated that the spectrum might be separated from the astronomical signal, based on the photometry of stars present in the field. It is the ambition of the team presenting this report to investigate this track.

Modtran versus real atmosphere

As already mentioned in section 1.1.2, strictly speaking, the validation of this approach is essentially limited to atmospheres that would behave as predicted by Modtran. Extensive observational validation of this still needed. We can however argue that the physics of molecular absorption for constituents like water vapour, ozone or molecular oxygen are well understood and modelled by Modtran, while the more fuzzy thermodynamic equilibrium of the atmosphere does not alter spectral absorption except via the number of molecules. (Thermal ray broadening and convection drifts have negligible effects). Nevertheless some tests of the capability of these models to reproduce the atmospheric alterations of real photometric data are still to be done.