OpenMARS ozone reference manual

Dataset summary

This dataset contains our analysis of the global atmospheric state of Mars over the specified time period through a synthesis of the Mars Global Circulation Model (GCM) used at the Open University and observational data taken by the Spectroscopy for the Investigation of the Characteristics of the Atmosphere of Mars (SPICAM) instrument in orbit around Mars. This product is useful as a reference global Martian atmosphere that has been constrained by observations.

For any queries on the dataset, please contact: openmars@open.ac.uk

Accessing the dataset

Along with the data files that make up this dataset, there is also a sample Python script that shows an interested user how the data in the files can be easily accessed. The plot that will be created if the supplied Python script (sample_data_plot.py) is run without modification will be identical to the plot shown in Figure 1. The supplied sample Python script can be modified to produce various plots of the different variables stored in the dataset (for some examples of the different plots available, a good place to start is to have a browse at https://matplotlib.org/gallery/index.html).

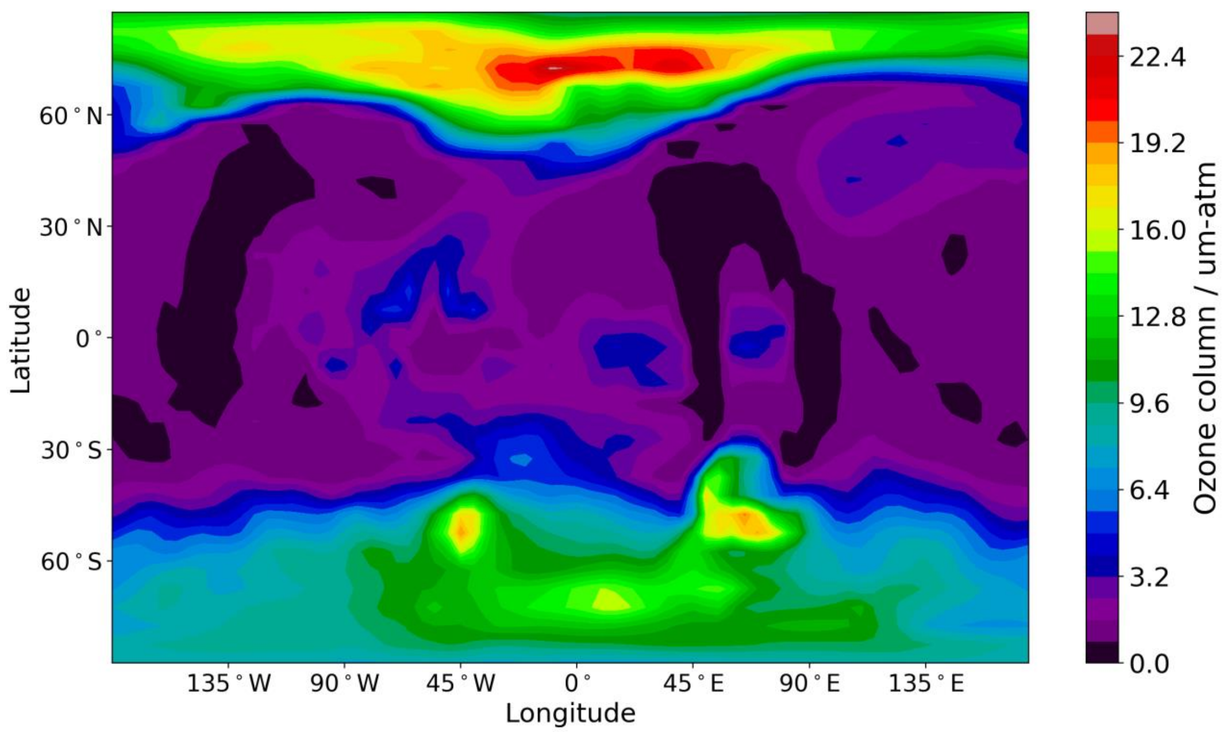

Figure 1 - Sample output of the ozone column abundance from the dataset created using the sample_data_plot.py script.

Structure of the reanalysis data files

This section details the structure of the files from the reanalysis which are made publicly available to interested users.

Dataset description

The ozone reanalysis produced covers just over one Mars year (L_S = 2˚ MY 27 to L_S = 68˚ MY 28), with any particular data file covering 30 sols. The data files are provided in netCDF4 format which are easily accessible by Python (see sample_data_plot.py for an example of how to access the data). The filename convention is as follows:

openmars_ozo_myMM_lsL_myMM_lsL.nc

where MM (27 or 28) indicates the Mars Year (MY) and L (0 to 359) the start/end value of solar longitude (to the nearest integer) for the period covered by the data file.

Dimensions

The dimensions of the reanalysis data files are listed in Table 1. The ozone reanalysis output in the data files depends on three dimensions (longitude, latitude, time) only. The horizontal grid spacing is 5˚ in both longitude and latitude. There were 35 vertical levels extending to an altitude of ~105 km used to create the data contained in this reanalysis product, although since the only additional assimilated observations were ozone column retrievals the reanalysis product contains only 2-D data.

Table 1 - Dimensions used for variables in the reanalysis data files.

Dimension	Number of values	Description
lon	72	Longitude
lat	36	Latitude
time	240	Time

The primary time variable used for each data file is the Martian sol (see Table 2 for all time variables). For ease of conversion and since the majority of the Mars science community use solar longitude and Mars year, these values are also included. The surface and atmospheric variables are output every 3 Martian hours starting at 3 a.m. on sol 2011 (sol 4 of MY 27), with sol 0 corresponding to L_S = 0˚ MY 24.

Table 2 - One-dimensional variables in each reanalysis data file.

Variable	Dimension	Description	Units
lon	lon	Longitude	Degrees east
lat	lat	Latitude	Degrees north
time	time	Martian Sol	Sols since 0.0
Ls	time	Solar longitude	Degrees
MY	time	Mars Year	NU

Atmospheric variables

The atmospheric variables included in each reanalysis data file are listed in Table 3. Only atmospheric variables that were assimilated into the MGCM are included in the final ozone reanalysis product.

Table 3 - Atmospheric variables in each reanalysis data file.

Variable	Dimension	Description	Units
o3col	lon, lat, time	Ozone column abundance	µm-atm

Overview of the components used to create the dataset

This section gives an overview of the three different components used to create the OpenMARS dataset, namely the Mars GCM, SPICAM observational data and the Data assimilation scheme that combines the two sources of information.

Mars GCM

The GCM used to produce this reanalysis product is the UK version of the LMD GCM (hereafter MGCM), which has been developed in a collaboration of the Laboratoire de Météorologie Dynamique, the Open University, the University of Oxford and the Instituto de Astrofisica de Andalucia. This model uses physical parameterisations shared with the LMD GCM, which are coupled to a UK-only spectral dynamical core alongside an energy and angular momentum conserving vertical finite-difference scheme. Tracers such as CO_2 and dust are transported by a UK-only semi-Lagrangian advection scheme (Newman et al., 2002) with mass conservation (Priestley, 1993).

The MGCM is similar to the model used in Montabone et al. (2014) for a previous reanalysis dataset but now includes additional sub-models. CO_2 is now transported as an additional tracer providing a better representation of the CO_2 cycle. A thermal plume model is used to better represent turbulent structures in the planetary boundary layer (Colaïtis et al., 2013), of importance for the evolution of tracers. A `semi-interactive' two-moment scheme is used to freely transport dust in the model (Madeleine et al., 2011), although the dust column optical depth at each grid point is scaled to match the observed dust distribution (Montabone et al., 2015).

The MGCM is also coupled to the LMD photochemical module (Lefèvre et al., 2004). The photochemical module provides multiple photolytic and chemical reactions with up-to-date reaction rates between 16 advected species including carbon dioxide, water vapour and ozone. It also includes heterogeneous processes removing odd hydrogen radicals, a process which has been shown to improve the agreement between models and observations (Lefèvre et al., 2008). Time-varying dust amounts are also taken into account in the photolytic reactions.

The model is truncated at wavenumber 31 resulting in a 5˚ physical longitude-latitude grid (and 3.75˚ longitude-latitude grid for the dynamical core) with 35 vertical levels extending to an altitude of ~105 km. The time-stepping regime for the physical and dynamical parts of the MGCM is 15 and 1.5 minutes respectively.

SPICAM observational data

This section describes the observational data available from the SPICAM instrument aboard the Mars Express (MEx) spacecraft. The SPICAM instrument on Mars Express is comprised of a dual UV/IR spectrometer. In the UV spectral range, it observed from 115–310 nm and is capable of ozone column density retrievals due to the strong Hartley band of ozone absorption around 250 nm. Even with the elliptical orbit, it was the first orbiting instrument capable of providing a global climatology with decent spatial and temporal coverage (Perrier et al., 2006).

SPICAM total ozone retrievals

The retrieval of total ozone from the Hartley band of intense absorption (220-280 nm) is described fully in Perrier et al. (2006), and briefly detailed in this section. The outcome of the retrieval process is just over 27,000 high signal-to-noise ratio observations for almost one and a half Martian years (L_S = 341˚ in MY 26 to L_S = 121˚ in MY 28). The SPICAM observational dataset is shown in Figure 2a, with the binned number of retrievals shown in Figure 2b.

The algorithm to retrieve the ozone column from the solar backscattered UV radiation in this version is a relative method, with the measured spectra divided by a reference spectrum, taken to be over Olympus Mons. This location is used since it is a region known to have extremely low ozone density values and minimal dust and aerosols in the atmospheric column owing to the low surface pressure and total column mass. The division by the reference spectrum filters out instrumental effects.

A forward radiative transfer model, containing assumptions on surface pressure, vertical ozone profile and temperature, is computed taking into account the geometry of the considered observation. The vertical distribution of dust follows the Conrath profile (Conrath, 1975) which was analytically derived from considerations of particle sedimentation and eddy mixing to vary the height that dust can reach in the atmosphere at different times of a Mars year. The a priori information is taken from the LMD GCM. A two-step method is used, with the model first computing the spectra assuming a dust-free atmosphere. For the second step, the modelled spectra are adjusted to the observed spectra by least square minimisation to retrieve the ozone column density, surface albedo and dust opacity, which are the three free parameters.

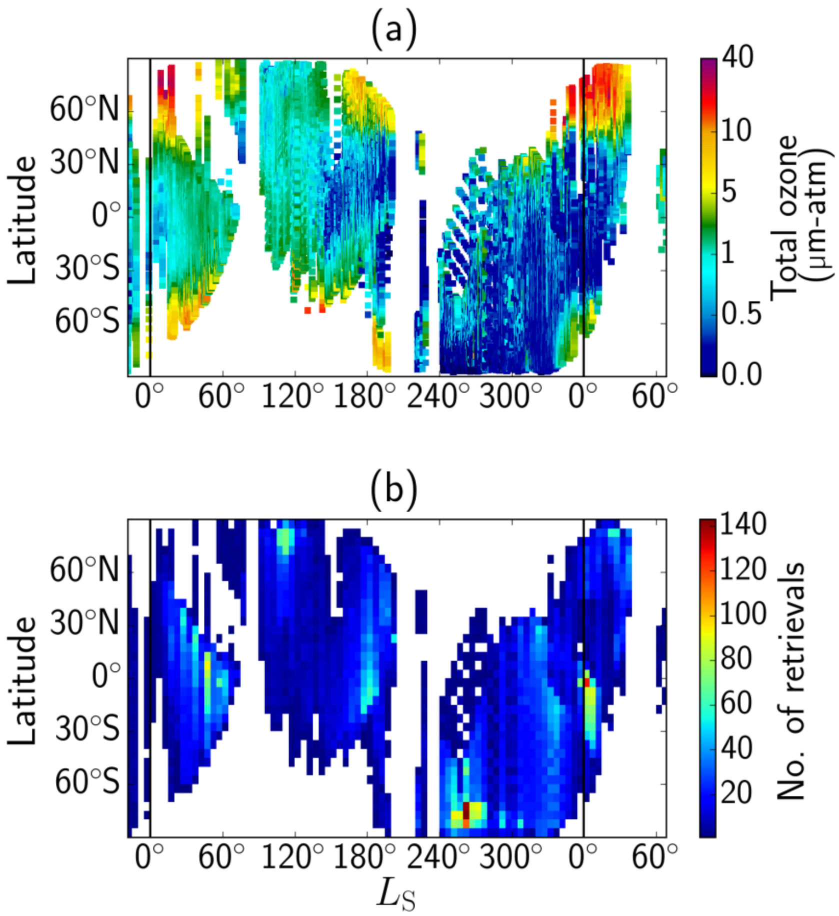

Figure 2 - SPICAM nadir retrievals for L_S = 341˚ MY 26 to L_S = 69˚ MY 28 as a function of latitude and solar longitude displaying a) the total ozone abundance and b) number of retrievals. The number of SPICAM retrievals are binned every 5˚ L_S and 5˚ latitude.

Quality control

To remove observations which have a low signal-to-noise ratio, observations with a solar zenith angle less than 85˚ and emission angle less than 30° are rejected. The relative method used does not currently take into account the effect of clouds, although any biases introduced due to the neglect of clouds was studied by Perrier et al. (2006). Using synthetic realistic spectra and the forward model, Perrier et al. (2006) find that the retrieval error increased to almost 100% with high cloud opacity ($\tau_{cloud} > 1$) but this occurs infrequently on Mars, with an average error of 10-15% in total ozone for more common thinner clouds (τ_{cloud} = 0.1-0.2). The ground resolution of the SPICAM observations at pericentre is around 4 km^2.

Before the SPICAM retrievals are assimilated into the MGCM, they are subject to further quality control measures. For the ~27,000 retrievals from SPICAM available, the relative sparseness of the data is an issue for a comprehensive buddy check algorithm, since there are not enough data points to be statistically significant over a sensible spatio-temporal region. A single spurious retrieval can have a large effect on the mean and standard deviation if there are only a handful of observations in the sub sample. Choosing a wide enough margin to get a statistically significant number of observations would require using observations from multiple days or over large degrees of latitude which would remove any natural variations in the retrievals. Each SPICAM retrieval R_i is instead compared to the retrieval $R_{i\pm1}$ either side of it in time. Spurious retrievals are then flagged up using three criteria; $|R_i - R_{i\pm1}| > 10$ µm-atm, $|L_i - L_{i\pm1}| < 5˚$ and $|S_i - S_{i\pm1}| < 1$ where L_i and S_i are the latitude and sol of observation i respectively. A value of 10 µm-atm was chosen to avoid rejection of retrievals which are realistic due to the sharp gradient on the boundaries of the high polar ozone abundance. Only 7 retrievals are found using this method, including retrievals of 38.97, 39.46 and 50.14 µm-atm at high southern latitudes in southern summer. These values are impossible since this region is in almost persistent daylight in southern summer and photolytic and chemical reactions with HO_x species, enhanced due to the sublimation of water vapour from the southern polar cap, prevent the total ozone from reaching anywhere near this level of ozone abundance.

Data assimilation scheme

To assimilate the observations, the MGCM uses the Analysis Correction (AC) scheme (Lorenc et al., 1991) adapted to Martian conditions. The AC scheme has previously been used to assimilate thermal and dust opacity retrievals from TES (Lewis & Barker, 2005) which are used to indirectly study the thermal tides. The dust opacity retrievals have also been used to perform a multi-annual study of interannual dust variability (Montabone et al., 2005, 2015), indicating localised regions which triggered the onset of the global dust storm in MY 25 and also found dust lifting by dust devils to contribute little. Observations during the TES aerobraking phase have been assimilated indicating an atmospheric warming at the onset of northern hemisphere winter due to the dust storm in MY 23 (Lewis et al., 2007). The AC scheme has also been validated against radio occultation (RO) measurements (Montabone et al., 2006), with the assimilation of TES thermal and dust opacity retrievals improving the agreement between the MGCM and the RO profiles. Recent work with the AC scheme has moved on to the assimilation of chemically passive water vapour and water ice (Steele et al., 2014a,b) to investigate the Martian water cycle and radiative effect of water ice clouds respectively and chemically active species such as ozone (Holmes et al., 2018).

The AC scheme is a form of successive corrections in which analysis steps are interleaved with each model dynamical time step. The modified successive corrections equation used by the scheme is

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{WQ}[\mathbf{y}_o - H(\mathbf{x}_b)]$$

where $\mathbf{x}_a$ is the analysis vector, $\mathbf{x}_b$ is the model background, $\mathbf{y}_o$ is the observation vector, H is the observation operator and **W** and **Q** are matrices of weights and normalization factors respectively. In each analysis step, the above equation is split into separate vertical and horizontal stages in order to spread the analysis increments from the observation locations to the surrounding model grid points. This is followed by the derivation of multi-variate increment fields for dynamical balance where applicable (e.g. after assimilating temperatures, geostrophic wind adjustments are applied).

Observations are inserted over an asymmetrical specified time window of 5 hours (four hours before an observations valid time until one hour after), optimally selected so that the assimilation will not unrealistically smooth out any inherent model variation. The asymmetrical time window is also used as it is beneficial because it biases the assimilation gains to regions ahead of the satellite ground track, which have not recently been observed. Spreading in time was also found to be beneficial in the case of relatively sparse data, where it is often better to use an observation from a slightly different time, with a reduced weight, rather than release the model. Full details on the assimilation method for ozone can be found in Holmes et al. (2018).

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