OpenMARS water 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 Thermal Emission Spectrometer (TES) 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 water vapour 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 water vapour reanalysis produced covers $L_S = 173^{\circ}$ MY 24 to $L_S = 186^{\circ}$ MY 25 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_vap_myMM_lsL_myMM_lsL.nc

where MM (24 or 25) 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 water vapour reanalysis output in the data files depends on three dimensions (longitude, latitude, time) only. The associated dynamical variables such as temperature and winds, can be found in the data products in the OpenMARS MY24-27 standard database, which has an identical structure in time and space. 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 water vapour column retrievals the reanalysis product contains only 2-D data.

Dimension	Number of values	Description
lon	72	Longitude
lat	36	Latitude
time	360	Time

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

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 2 Martian hours starting at 2 a.m. on sol 361 of MY 24, with sol 0 corresponding to $L_S = 0^{\circ}$ 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. The atmospheric variables of temperature and dust column are not included in the final water vapour reanalysis product, as they can already be found in the OpenMARS MY24-27 standard database. Therefore, the only assimilated atmospheric variable in the water vapour reanalysis product is the water vapour column.

Variable	Dimension	Description	Units
vapcol	lon, lat, time	Water vapour column abundance	kg m⁻²

Table 3 - Atmospheric variables in each reanalysis data file.

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, TES 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 CO₂ 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. CO₂ is now transported as an additional tracer providing a better representation of the CO₂ 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.

TES observational data

This section describes the observational data available from the TES instrument aboard the Mars Global Surveyor (MGS) spacecraft. The TES instrument operates in the thermal infrared between 6– 50 μ m (200-1600 cm⁻¹). The spectrometer began its mapping operations on 1 March 1999 ($L_S = 104^\circ$, MY 24) and ended on 31 August 2004 ($L_S = 81^\circ$, MY 27). MGS completed 12 orbits each sol, creating two sets of 12 narrow strips of data, running roughly north-south and separated by ~30° in longitude. The two sets of data contain observations at local times around 2 a.m. and 2 p.m. respectively, with the variation larger near the poles (for example, in the polar regions the daytime observations range between 12:30–14:30). While TES temperature profiles and dust opacity retrievals are assimilated in the water vapour reanalysis dataset, full details on these retrievals can be found in the OpenMars-MY24-27-reference-manual accompanying the OpenMARS MY24-27 standard database.

TES water vapour retrievals

The only water vapour column data currently available for assimilation into the MGCM are from the TES instrument aboard the MGS spacecraft. Water vapour column retrievals are obtained by comparing synthetic spectra with TES spectra from rotation bands in the 28–42 μ m region. In this region, the TES signal-to-noise ratio is relatively high, and the contribution to the spectrum from water vapour can easily be separated from the dust, water ice and surface contributions (Smith, 2002).

When calculating the synthetic spectra, water vapour is assumed to be well mixed up to the condensation level, and zero above. The estimated uncertainties in the vapour column abundance caused by random errors are 5 pr- μ m, while uncertainty in the pressure broadening of water vapour by CO₂ results in a systematic error likely to be much less than 25%.

Quality control

Full details of the quality control are in Steele et al. (2014b), and are briefly reported here. Because of the restrictions of the retrieval algorithm, water vapour retrievals are only provided for locations where the surface temperature is greater than 220 K, which excludes data from the nighttime orbits and over the winter polar regions. The number of TES retrievals varies with time, but in full operational mode each strip of data typically contains ~700 retrievals, spaced ~0.15° (10 km) apart in latitude. The TES instrument retrieved approximately 13 million water vapour columns during its lifetime, with the number of retrievals binned into discrete latitude-time periods shown in Figure 2, although this dataset currently only includes retrievals from $L_S = 173^\circ$ MY 24 to $L_S = 186^\circ$ MY 25.

For the vapour column observations, the variation with latitude can be quite large due to differences in topography and temperature, but nearby measurements should conform to within a specified threshold. To investigate possible spurious observations, a buddy-check was applied on each strip of data after all retrievals had been scaled to the 610 Pa pressure level to remove the effects of topography. For each observation, the buddy-check compares the value to the mean of all the observations within a specified meridional distance d either side of it. The observation is highlighted as a possible error if its value differs by some threshold value δ_{vap} . As the vapour column is strongly dependent on latitude, applying a buddy-check with values of d too large removes observations with natural variation. Conversely, values of d too small results in too few observations to perform a meaningful statistical analysis. Numerous tests showed that comparing observations over a distance d = 300 km (~5° in latitude), and excluding any observations where $\delta_{vap} > 3\sigma$ (around 4–10 pr-µm depending on location and season) from the mean, gave the best combination of (1) a large enough sample of data for comparison, (2) the removal of spurious observations and (3) the retention of observations with natural variation. Only a small fraction of the water vapour column observations are discarded (~0.5%) by the buddy-check algorithm and so it does not negatively impact on the amount of data available for assimilation.



Figure 2 - Number of retrievals of TES water vapour column in 2 sol by 5° latitude bins. Dashed vertical lines indicate the end of a Mars year. White indicates no data available in this particular bin.

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

$$\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{W}\mathbf{Q}[\mathbf{y}_{o} - H(\mathbf{x}_{b})]$$

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 \mathbf{W} and \mathbf{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 6 hours (five 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 water vapour can be found in Steele et al. (2014b).

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