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Photochemical model of the Martian atmosphere to investigate the fate of trace gases

P. Witek (1), P. Wajer (1), M. Banaszkiewicz (1), W. Kofman (1,2), L. Czechowski (3) and A. Pommerol (4)

(1) Space Research Centre PAS, Warsaw, Poland (wajer@cbk.waw.pl), (2) Institut de Planetologie et d'Astrophysique de Grenoble CNRS/UJF, Grenoble, France, (3) Institute of Geophysics, Faculty of Physics, University of Warsaw, (4) Physics Institute, Space Research and Planetary Sciences - University of Bern, Bern, Switzerland.

Abstract

The European-Russian ExoMars Trace Gas Orbiter (TGO) is now on its scientific orbit. The orbiter has started to return new data on abundance of trace gases as well as colour and stereo images of the surface, that are useful in characterizing the sources and sinks of some atmospheric gases. One of the most interesting subjects of investigation is appearance and disappearance of large quantities of methane (CH_4) on Mars on short timescales. Our model of Martian atmospheric photochemistry, chemistry and transport is developed to analyse the data sent back by the probe. All constituents of the atmosphere are subjected to solar radiation and react with each other, in presence of the atmospheric aerosols. This leads to several hundred reactions that change the abundance of different species. We model these reactions in single-column model coupled with model of the subsurface, to properly simulate the release, transport and loss of trace gases. The molecules can react with each other, be exchanged between the layers of the atmosphere and may be lost to reactions with aerosols and surface, or escape into space.

1. Introduction

Changes in the abundance of trace gases in the atmosphere indicate active processes on a planet. In the last 15 years Earth-based observatories, Mars Express Orbiter and MSL Curiosity rover detected appearance of methane in the Martian atmosphere [1][2][3]. The data show high variability, suggesting occasional release of gas and removal on timescales much shorter than expected from photochemistry alone. The sources of this gas are of special interest because they may signify recently active hydrothermal, volcanic or biological processes. The variability currently lacks undisputable explanation, and sinks capable of reducing the concentration to the background level on the scale of several months are not known.

The release of other trace gases together with methane may be an indicator of its origin. If methane is accompanied by sulphur dioxide, it suggests the release of volcanic gases. A likely source of methane on Mars is hydrothermal alteration of silicates (serpentinization) in the subsurface, and biological origin through methanogenesis (whether by extant or extinct microorganisms) is not excluded. Methane can also be released from methane hydrates in the permafrost, where it could have been trapped after formation in the past. [1]

Recent tumbling experiments have shown that wind erosion of quartz and basalt grains in the absence of oxygen activates the surface and leads to production of reactive species [4][5]. The ubiquity of dust on Mars makes this possibly important sink for methane, which can be lost due to formation of strong covalent bonds between silicon and methyl group [4]. Heterogeneous reactions on dust and ice aerosols in the Martian atmosphere have been previously suggested to be important for loss of some species [6].

High precision measurements of trace gases, now possible with instruments such as NOMAD and ACS on board ExoMars TGO, will determine the amount of various trace gases, including detection or at least placing strong constraints on abundance of species that have been predicted to be present, but not yet detected in the Martian atmosphere (e.g. SO_2) [7][8].

2. Research methodology

We develop a single-column model of the Martian atmosphere to compute its steady-state chemical composition. Starting there, we will study the release, propagation and loss of trace gases such as methane and other hydrocarbons, and sulphur and chlorine species. To model the transport we solve one-dimensional time-dependent equations:

$$\frac{\partial n_i}{\partial t} = \frac{-\partial \Phi_i}{\partial z} + P_i - n_i L_i \qquad (1)$$

Where n_i is the concentration of i-th molecule (cm^{-3}), Φ_i is the vertical flux of molecules ($cm^{-2}s^{-1}$), z is the altitude, P_i is the production rate ($cm^{-3}\ s^{-1}$), and L_i is the loss rate (s^{-1}).

We model molecular and turbulent diffusion of the molecules and changes of their concentration resulting from interaction with each other and solar radiation. We simulate changes in the concentration resulting from chemical reactions, including some important heterogeneous ones. We use two-stream approximation of the radiative transfer equation. The overall photon flux is the sum of the direct and scattered parts. We simulate temporal variability of the incoming radiation, absorption and Rayleigh scattering by gas molecules and scattering on aerosol particles such as dust or ice crystals.

Our photochemical model requires upper and lower boundary conditions for each molecule. We include the loss of some molecules to space at the upper boundary, especially for the lightest species such as H or H_2 [9]. The lower boundary conditions are more complex. The molecules may react with chemically active surface and in some cases (like methane) may be released from the subsurface. This requires knowledge and proper modelling of the processes in the subsurface.

Separate numerical model is developed to simulate the processes in the Martian subsurface such as diffusion through porous rocks, adsorption and desorption, and others. The model will be coupled with the main photochemical model of the atmosphere.

We plan to use images obtained by the Colour and Stereo Surface Imaging System (CaSSIS) on board the ExoMars TGO [10] to put proper lower boundary conditions on our atmospheric model and numerical model of the subsurface. For example colour images obtained by CaSSIS should give us information on mineralogy of the surface in places where the methane release is most likely.

3. Summary and Conclusions

With the sophisticated instruments on board the Trace Gas Orbiter studying Martian atmosphere and surface, an adequate model of transport and changes of the concentration of the trace gases is needed. We develop a complex chemical and photochemical model to simulate the transport and fate of the gas species that are known to be present or expected to be detected in the Martian atmosphere. The behaviour of elusive trace gases such as CH_4 holds information on past and present activity and habitability of Mars. The results of our simulations will be confronted with measurements to assess the importance of various considered mechanisms of loss.

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