Influence of the Martian regolith on the atmospheric methane and water vapour cycle

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Abstract

Context. The Martian methane and water cycle are subject of ongoing research through simulation. Exchange with the subsurface has a potentially strong impact, but is often neglected.

Aims. For methane, I determine if adsorption with an increased enthalpy can explain the observed seasonal variations and conflicting observations by the Trace Gas Orbiter and the Curiosity rover. For water, the impact of adsorption and ice formation in the subsurface on the global cycle is studied. A new way of initializing the soil, by running a decoupled subsurface model, is tested. Depths of stable subsurface ice and subsurface water distributions are studied.

Methods. A General Circulation Model (GCM) is used with a purely diffusive subsurface model. For methane, different initial states, source scenarios, and decay times are tested. For water, a model without an active atmosphere is implemented to provide an initial state. The effect of the subsurface with this initial state on the full atmospheric water cycle is tested.

Results. For methane, a strong influence on the global methane cycle is observed. Seasonal variations measured at Gale Crater are reproduced, but the conflicting observations cannot be explained by adsorption. For water, the new initialization can be used without completely disrupting the water cycle. It leads to a generally wetter atmosphere, in conflict with observations. Found ice table depths do not match well with observations, but ice profiles reproduce previous findings.

Conclusion. Methane adsorption is able to partly explain observed variations, but cannot be the only process to influence methane abundances. The new initialization method for water works well in principle, but a more refined model is needed for more realistic results.
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1 Introduction

The work presented here focuses on the exchange of the Martian soil, also known as regolith, with the atmosphere and on two molecules of great importance for the study of Mars: methane and water. For both molecules, the subsurface has a potentially strong impact on the global distribution and transport. Through the means of 3D climate simulations the influence of the soil on the global cycle is studied. In this introduction I first present the current climatic conditions on Mars. I then explain the process of adsorption in the soil as well as go over the reasons for the importance of the two molecules, their history of observations, and current open questions. I also present the type of climate model used.

1.1 Martian Climate

The Martian climate is a very interesting subject of study, both as comparison to the Earth’s and in its own right. An extensive overview is presented by Haberle et al. (2017). Mars is similar to Earth in some regards like rapid rotation and a seasonal climate. One Martian day, called “sol”, is about 24 hours and 40 minutes long and its rotational axis is tilted by about 25° relative to its orbit. At the present time the Martian orbit is slightly eccentric, with an eccentricity of 0.09, and a Martian year lasts about 669 sols or 687 Earth days. Numerical simulations have shown that the planets inclination and eccentricity change chaotically over time due to the gravitational interaction with the other planets, with important implications for the climate. This happens on time scales on the order of a few hundred thousand years (Laskar, 1994, 2003).

The atmospheric composition and pressure on Mars are very different from Earth. The main constituent gases by volume are carbon dioxide (CO$_2$) with 94.9%, nitrogen (N$_2$) with 2.79%, and Argon (Ar) with 2.08% (Franz et al., 2017). The surface pressure is much lower than Earth’s and has strong variations. Typical values lie between 600 and 1000 Pa, less than 1% of typical Earth surface pressures (Harri et al., 2014).

The temperatures are much lower on Mars than on Earth, ranging from about
300°K during the summer in some locations down to about 148°K during the winter near the poles. With temperatures so low, the CO$_2$ in the atmosphere condenses and forms a seasonal polar cap (Neugebauer et al., 1971; Martínez et al., 2017).

1.2 Adsorption

Adsorption is a process in which one or multiple layers of molecules stick to the surface of a substrate, mostly by Van der Waals forces and without chemically reacting with it. As such, adsorption is fully reversible. The amount of adsorbed material is increased by low temperatures and high surface areas. This makes adsorption potentially very important in the Martian soil, which is relatively cold and likely has a high surface area per unit mass, also known as specific surface area (SSA).

The exact behaviour of adsorption is usually described by a curve called isotherm. It shows the amount of gas adsorbed depending on the ratio of partial pressure and saturation pressure for a specific temperature and material. It often has two regimes, one for high and one for low partial pressures, which can be attributed to the formation of single or multiple layers of adsorbed gas (Brunauer et al., 1938). For very small partial pressures, the relation between partial pressure and adsorbed amount is linear and can be modelled like in Equation 1 below, with an exponential dependence on temperature and enthalpy of adsorption onto the surface material (Gough et al., 2010).

\[
\text{n}_{\text{ads}} \propto n_{\text{gas}} \cdot \text{SSA} \cdot \exp \left( \frac{\Delta H}{RT} \right)
\]

(1)

Here $n_{\text{ads}}$ is the amount in the adsorbed phase, $n_{\text{gas}}$ is the amount in the gas phase, SSA is the specific surface area, $\Delta H$ is the enthalpy of adsorption, $R$ is the universal gas constant, and $T$ is the temperature.

1.3 Methane

In this section, the question of the importance of methane is addressed, followed by its detection history and currently open questions.
1.3.1 Importance of Methane

Methane is destroyed by photodissociation in the upper and oxidation in the lower Martian atmosphere. Its lifetime is estimated to be \(\sim 300\) Earth years by photochemical models. This is much longer than on Earth, where the lifetime is about 10 years (Voulgarakis et al., 2013), but still very short compared to geological timescales. Therefore, any methane detected on Mars must have entered the atmosphere in the recent past, either by a continuous flux or a recent emission event (Lefèvre and Forget, 2009).

So far it is unknown if and what kind of methane sources exist on Mars, but different scenarios have been proposed. It can be produced by geological processes in the Martian crust (Neal and Stanger, 1983) or brought in by comets and other material from outside (Schuerger et al., 2012). Another possible but unlikely source could be microbial life, which is the main source of methane on Earth (Weiss et al., 2000). Understanding the sources and behaviour of methane on Mars will bring important insights about the present and past conditions on the planet.

1.3.2 Detection History

The first tentative measurement of methane on Mars was done by the Mariner 9 spacecraft with its infrared spectrometer, but with an uncertainty in the range of the measured value (Maguire, 1977). Twenty years later a measurement from Earth detected the gas with a value similar to Mariner 9, but also with similar uncertainty. Even though there is a lot of methane in Earth’s atmosphere, its lines can theoretically be distinguished from Martian lines using the Doppler shift caused by the relative velocity between Earth and Mars on their orbits (Krasnopolsky et al., 1997). This result was later improved upon by another measurement from Earth, giving the first low uncertainty detection with 10±3 parts per billion by volume (ppbv) (Krasnopolsky et al., 2004).

The first low uncertainty detection by a spacecraft was done by Mars Express with its Planetary Fourier Spectrometer, which measured 10±5 ppbv (Formisano et al., 2004). Another measurement from Earth observed a re-
gional plume which quickly disappeared again (Mumma et al., 2009). Global mapping was done and regional differences were found by the Thermal Emission Spectrometer on board the Mars Global Surveyor spacecraft, with values between $5 \pm 2$ ppbv and $33 \pm 9$ ppbv (Fonti and Marzo, 2010).

With the landing of the Curiosity rover in 2012 and its Tunable Laser Spectrometer (TLS) a new level of precision was reached. It measures absorption of a laser at 3.3 $\mu$m wavelength, which is sent 81 times through a sampling chamber. The chamber can either be filled directly from the atmosphere or through a scrubber, which removes CO$_2$ and thereby concentrates any trace gases. It found an average background level of $0.41 \pm 0.16$ ppbv and a spike in methane, averaging $7.19 \pm 0.74$ and lasting 60 sols (Webster et al., 2015, 2018). Continued measurements by TLS revealed seasonal variations of the methane background (Webster et al., 2018). The values are shown in Figure 1 in dependence of solar longitude. The solar longitude is a frequently used measurement of time on Mars. It describes the orbital Mars-Sun angle as measured from the northern hemisphere spring equinox. One Martian year therefore lasts 360 degrees solar longitude. The spike measured by Curiosity was later confirmed through a reanalysis of Mars Express data, marking the first independent confirmation of a methane detection (Giuranna et al., 2019).

There also have been some notable non-detections of methane, for example from Earth by Villanueva et al. (2013) placing a $3\sigma$ upper limit of 6.6 ppbv. More recently the first results from the Trace Gas Orbiter were published, which has two instruments for the measurement of methane. They measure trace gases by spectroscopically analysing sunlight that has passed through the atmosphere during sunset or sunrise. On the one hand, this makes measurements low in the atmosphere difficult, due to relatively high atmospheric opacity from dust. On the other hand, the very long path length and bright light source increase the possible sensitivity by orders of magnitude compared to previous instruments. However, there was no methane found anywhere on the planet, placing upper limits of 0.05 ppbv and even lower in some locations (Korablev et al., 2019). A comparison with the measurements from Curiosity can be found in Figure 1.
Figure 1: Methane measurements by Curiosity over the martian year in solar longitude and upper limit from the Trace Gas Orbiter (Webster et al., 2018; Korablev et al., 2019).

1.3.3 Open Questions

Currently the most sensitive measurements are from TGO and they are in conflict with the also quite sensitive measurements from Curiosity. So far, there has not been a measurement by TGO directly over Gale Crater, the location of Curiosity, but methane should be mixed relatively evenly around the planet given it’s photochemical lifetime of about 300 years. In the case that the measurements from both are correct, there has to be a physical process that removes the methane from the atmosphere at a rate about 1000 times faster than the destruction through photochemical reactions (Korablev et al., 2019). The potential nature of such a process is unknown. In this work I investigate if adsorption in the soil can explain these discrepancies.

A similar problem arises with the detection of extended plumes and regional differences in methane concentration. It is unknown how these regional differences can exist in the quickly mixing martian atmosphere and how the plumes can disappear as quickly as suggested by the measurements.
The seasonal variations measured by Curiosity are also of unknown origin, since no known atmospheric process can explain them (Lefèvre and Forget, 2009). There have been recent simulations by Moores et al. (2019) suggesting the observations could be explained by adsorption, when assuming a very high enthalpy of adsorption. These simulations were carried out with an one dimensional model, making assumptions about the exchange with the rest of the atmosphere. In this work I investigate this scenario further, using a three dimensional model of the whole planet.

1.4 Water

In this section, the question of the importance of water is addressed, followed by a discussion of evidence for its existence on Mars and currently open questions.

1.4.1 Importance of Water

On Earth liquid water is essential for all forms of life. If there is life as we know it on Mars, it will also be bound to its presence. However, the current surface temperatures and pressures are highly unfavourable for the presence of liquid water, since they are usually below the triple point (Smith, 2008).

As mentioned before, Mars undergoes relatively frequent changes in its orbital parameters. This triggers the redistribution of water ice around the planet which is one of the few geological processes that still shape the surface of the Planet. Understanding the behaviour of water is essential for understanding this process (Mellon and Jakosky, 1995).

There is ample amount of evidence that, throughout its history, Mars had large amounts of liquid water and water ice. Understanding the water is therefore not only important to understanding the present, but also the past of Mars (Carr, 1986).

The water in the Martian atmosphere is also of great importance for its climate. Clouds of water ice can form over large parts of the planet, changing the
temperature structure inside the atmosphere by interacting with the sunlight coming in and the infrared radiation emitted by the surface. They also influence the dust, since the grains serve as nucleation sites and can subsequently be removed from the atmosphere by snowfall (Clancy et al., 1996; Madeleine et al., 2012).

An additional aspect of water is human exploration. If humans want to stay on the surface of Mars for extended periods of time, it will be impractical to bring all the necessary water with them from Earth. Finding suitable reservoirs of water will therefore be of great importance for such a mission (Hoffman and Kaplan, 1997).

1.4.2 Evidence for Water on Mars

Since the first detection through spectroscopy from Earth by Spinrad et al. (1963) and from a spacecraft by Mariner 9 (Conrath et al., 1973), water has been found on Mars in many forms and places, as presented in an extensive overview by Lasue et al. (2019).

![North polar ice cap as seen by the Mars Global Surveyor spacecraft. Credit: NASA/JPL/Malin Space Science Systems.](image)

The largest visible reservoir of water today is the north polar cap, seen in Figure 2, which consists primarily of water ice. It has a diameter of about 1100 km and shows very few craters, suggesting a possible surface age as low as 1500 years (Landis et al., 2016). The corresponding south polar cap has a much smaller extend with ca. 400km, but is of similar volume (Plaut et al.,
It is covered by a thin layer of CO$_2$ ice all year round. Together the two caps contain water equivalent to a global layer of 22 meters (Carr and Head, 2015).

There is a lot of geomorphic evidence for ground ice, seen first by the Viking orbiter. Creep deformation of ground ice enables a quasi-viscous relaxation of the topography, causing features like concentric crater fill and terrain softening (Squyres and Carr, 1986). Ground ice has also directly been observed by the Phoenix Lander. It found pure water ice after digging into the soil at its high latitude landing site (Smith et al., 2009).

The Gamma-Ray Spectrometer and the Neutron Spectrometer on board the Mars Odyssey orbiter were able to detect hydrogen in the upper decimetres of the martian surface, which was interpreted as the presence of water. They have measured large amounts of water equivalent hydrogen throughout the high latitudes of both hemispheres, indicating large reservoirs of ground ice. They also detected some amount of hydrogen at low latitudes whose nature is still debated (Feldman et al., 2004; Pathare et al., 2018).

While the conditions are unfavourable for stable liquid water, transient liquid water has been observed in the form of recurring slope lineae. These are narrow dark markings on steep equator facing slopes that appear during warm seasons and fade again during cold ones. They are most likely caused by extremely salty water (McEwen et al., 2011; Chevrier and Rivera-Valentin, 2012).

Despite the presence of such large amounts of water ice, the martian atmosphere is very dry. Its water content is usually measured in precipitable micrometers (the thickness of the water layer if all the water were at the surface) with local values ranging between close to zero and 100 and global averages between 5 and 20 (Jakosky and Farmer, 1982; Smith, 2002). One precipitable micrometer is equivalent to one gram of water per square meter.

### 1.4.3 The Current Water Cycle

The current water cycle is dominated by the north polar cap. In the northern summer it releases large amounts of water vapour, which is then transported
south by the global Hadley cell circulation. Most of the released water stays in the northern hemisphere and gets eventually transported back to the north pole. The back transport happens through repeated sublimation and condensation of water as the seasonal ice cap retreats during the northern spring (Richardson and Wilson, 2002). The south polar cap also releases some water, but far less in comparison. Overall, this causes a strong asymmetry between the hemispheres, with the northern one being much wetter. All of this can be seen in the observations by Mars Global Surveyor in Figure 3, showing longitude averaged water vapour column densities over solar longitude.

![Figure 3: Longitude averaged water vapour observed by the Thermal Emission Spectrometer on board the Mars Global Surveyor spacecraft (Smith, 2002, 2004, 2006).](image)

1.4.4 Questions about the Soil

Ground ice and adsorbed water must be in exchange with the atmosphere through diffusion. In spite of this, current models of the martian climate are able to reach relatively good agreement with observations of the global water cycle without taking the subsurface into account (Navarro et al., 2014). However, previous studies found that it might be possible to reach significant improvements by integrating a subsurface model (Böttger et al., 2005). The objective of my work is to perform this integration for the used model.

While there are models that study water in the soil and they are able to reproduce the distribution of subsurface water, when it comes to the amount
of water in the soil they do not match the observations well. An improvement in the used isotherms might be able to provide a solution to this problem (Steele et al., 2017).

So far it is also unclear how exactly the subsurface ice at high latitudes got there, how it evolved over time, and if it is currently in equilibrium with the atmosphere. The nature of the hydrogen found at low latitudes is also unknown, since ice is not stable there. Hydrated minerals have been proposed as an explanation (Fialips et al., 2005), but part of it could also be explained by adsorbed water.

1.5 General Circulation Models (GCMs)

GCMs are climate models which simulate the atmospheric dynamics by directly calculating the Navier-Stokes-Equations and combining them with various physical and chemical processes. By doing so they are able to provide a complete three-dimensional and time-dependent atmospheric state. They were first developed for simulations of the Earth’s atmosphere and are used for weather forecasting and climate studies. Later they were adapted to Mars and other planets of the solar system with great success (Forget et al., 1999).

The model used in this work is the GCM developed by the Laboratoire de Météorologie Dynamique (LMD) in Paris. It is written in Fortran and is developed and improved since the early 1990s. It splits the calculations into a dynamical and a physical part. The dynamical part solves the equations for the atmospheric circulation and is shared between the models of all terrestrial planets. The physical part calculates the physical equations specific to the planet on each gridpoint.

The model is continually improved by implementing new and more precise physical processes like water and CO$_2$ ice cloud microphysics, sub-grid scale clouds, improved dust treatment, and improved resolution (Navarro et al., 2014; Pottier et al., 2017; Vals et al., 2018). Since a few years it has reached a level of accuracy that allows its use in engineering and scientific work whenever direct observations are not available (Millour et al., 2015).
2 Methodology

In the following, I describe the atmospheric model used in more detail as well as the specific subsurface implementations for methane and water. I also talk about the computing infrastructure I had access to.

2.1 GCM

Two different versions of the LMD GCM where used in this work. For the simulations of Methane it is based on the version from 2009. This version was used because it was available from the very beginning of the project. The physical parametrization includes radiative transfer (including contributions from dust and non local thermodynamic equilibrium), turbulent diffusion, convection, effects of topography and gravity waves, subsurface thermal conduction, and CO₂ condensation. It also simulates atmospheric tracers and their transport, sources, and chemistry (Millour and Forget, 2018). It runs with a spatial resolution of 64x48x25 (longitude x latitude x altitude) covering the whole planet and extending up to 100 km altitude. The timestep is 1.5 minutes for the dynamics part and 30 minutes for the physical part.

For the simulations of water the most recent version of the LMD GCM from 2019 is used. It features many improvements in various areas including radiatively active ice clouds, cloud microphysics and greatly improved dust treatment (including dust pickup, transport, size prediction, gravitational sedimentation, and scavenging by water and CO₂ snowfall). It also includes the possibility of parallel execution. This is of great importance, since the computational cost rises by about a factor of three compared to the methane model. This is not only caused by the additional physical processes, but the accurate prediction of the water cycle also requires improving the vertical resolution to 32 layers and decreasing the physical timestep to 15 minutes. These improvements also come with significant changes to the underlying structure of the code, requiring adaptations in the implementation of the subsurface and in the way the simulation is run.
2.2 Methane

Here I describe the subsurface model used as well as details of the initialization and the implementation of water ice and possible methane sources. I also give an overview of the performed methane simulations.

2.2.1 Subsurface Model

The subsurface parametrization is based on the work from Meslin et al. (2011) and summarized here. It uses a purely diffusive model, coupled to the model of thermal conduction in the soil. There are 18 subsurface layers and the layer thickness is scaled exponentially down to 26 meters as illustrated in Figure 4. The exact depths and the formula used can be found in Table 2 in the Appendix.

![Subsurface Model Diagram](attachment:image.png)

**Figure 4:** Schematic view of the subsurface models layer structure for three gridpoints. Subsurface shown in brown, first atmospheric layer shown in blue. Layers close to the surface are too thin to see.

The calculation of the subsurface behaviour of methane is done with an implicit time-marching scheme and together with the calculation of turbulent diffusion in the overlying atmosphere. The two reservoirs are free to exchange gas as long as the surface is not covered with CO$_2$ or water ice, in which case a zero flux boundary condition is imposed. At the bottom a zero flux boundary condition is prescribed, unless a source flux from below is activated. Direct exchange between the soil layers of different gridpoints is not possible, only
the atmosphere can perform transport between gridpoints. The conditions in
the soil are in between the regimes of molecular diffusion (where the collisions
between the molecules dominate) and Knudsen diffusion (where the collisions
with the surrounding material dominate). Therefore an interpolation between
the two is used. If there is water ice partly filling the pores of the soil, this
also taken into account by reducing the diffusion coefficient.

The amount of adsorbed gas is modelled through fluxes of adsorption and
desorption, taking into account the kinetics of the adsorption process. This
includes dependence on temperature, specific surface area of the soil, and
methane concentration in the air.

Some of the processes or parameters used for the calculations are only poorly
constrained by lab experiments and observations. Others come with difficulties
in the implementation. Therefore, the following assumptions are made:

- Any advection of gas in the soil is negligible. Diffusion is the only trans-
  port process.
- Pressure in the soil is constant with depth and equal to the current
  surface pressure.
- The specific surface area, porosity without water ice, tortuosity, soil
density, and enthalpy of adsorption are constant over the whole planet
  and with depth.
- The presence of water ice has no effect on the strength of adsorption or
  available surface area. Only the diffusion speed is affected.
- Adsorption never leaves the linear regime, therefore all results are scal-
  able by overall methane concentration.
- Thermal conductivity is constant with time and depth at each gridpoint.
- If destruction of methane in the atmosphere is calculated, it is constant
  over the whole planet.

Other parameters are treated as free parameters and their effect on the simu-
lation is investigated. These are the atmospheric decay time, the enthalpy of
adsorption, and the specific surface area. In the simulations by Meslin et al. (2011), a value of 18.08 kJ mol$^{-1}$ was used for the enthalpy of adsorption, based on lab experiments by Gough et al. (2010). This resulted in only minor effects on the methane cycle compared to the case without adsorption. In a later 1D study Moores et al. (2019) were able to reproduce the seasonal variations observed by Curiosity in Gale Crater by using a much higher value for the enthalpy of 31.5 kJ mol$^{-1}$. Based on this result I perform my simulations with the higher value.

For the specific surface area a value of 17 m$^2$/g is the default, based on measurements from the Viking lander (Ballou et al., 1978). Higher values of 100 m$^2$ are also tested to study the effect of very strong adsorption. Most simulations were performed without any decay to simplify interpretation of the results. A very fast decay with day decay time was used a few times to find out if such a process could confine the methane distribution around a source.

Since observations from TGO placed very strong limits on the global abundance of methane, it effectively excludes the possibility of a global methane cycle. Most of the methane simulations done in this work were already completed at the time of publication of this data and therefore have to be interpreted under the assumption that the TGO results are wrong.

### 2.2.2 Initialization

The atmosphere, except for the methane abundance, is initialized to a state taken from a multi year simulation by Meslin et al. (2011), which had developed a repeatable yearly cycle. For methane a uniform initial distribution in the atmosphere is generated. Since the atmospheric processes are relatively fast, the only really important parameter is the average methane concentration. Initializing the adsorbed methane in the soil is more difficult, since adsorption is temperature dependent and the soil is a much larger reservoir than the atmosphere in terms of storage capacity. The available program initializes the adsorbed methane according to the yearly average temperature, which should lead to an initial state relatively close to equilibrium. However,
this assumes constant exchange between the atmosphere and subsurface and does not take the effect of the seasonal CO$_2$ polar cap into account. The consequences of this are described in Section 3 and lead me to initialize the soil with a lower average methane concentration than the atmosphere in order to reach global equilibrium faster.

There were also simulations performed without any methane in the soil. These show how quickly the soil is able to take up methane and are used to determine an apparent atmospheric lifetime caused by this uptake.

2.2.3 Implementation of Water Ice

The methane simulations do not contain any dynamic water and therefore cannot simulate the build-up or disappearance of ground ice. However, the presence of water ice has a very significant effect on the diffusion speed, because it fills up the pore space and decreases the cross-section available for diffusion. For this reason, I added ground ice based on data collected by the Mars Odyssey’s Neutron Spectrometer and published by Pathare et al. (2018). A very simple ice profile is assumed. The ice fraction is equal to the measured one in all layers below the measured ice table depth, which is the shallowest depth where water ice is stable. Once initialized, the water ice content stays constant and does not change with the seasons or over the years.

2.2.4 Sources

I test different implementations and scenarios of methane sources. In the model, methane can be injected from below into the deepest layer, inside the top layer, or directly into the first layer of the atmosphere. This can be done for one gridpoint or an arbitrarily defined square. The source can be activated continuously or as a spike emission for a limited amount of time.

2.2.5 Overview over Performed Simulations

Table 1 on page 16 lists all methane simulations presented in Section 3.
Table 1: Overview over the methane simulations presented in this work.

<table>
<thead>
<tr>
<th>name</th>
<th>settings</th>
<th>purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>“high enthalpy”</td>
<td>high enthalpy, atmospheric methane: 50 pptv, soil methane: 30 pptv, no source, no decay</td>
<td>reaching equilibrium, study time and space variations induced by the soil</td>
</tr>
<tr>
<td>“low enthalpy”</td>
<td>low enthalpy, atmospheric methane: 0.5 ppbv, soil methane: 0.2 ppbv, no source, no decay</td>
<td>reaching equilibrium, study time and space variations induced by the soil</td>
</tr>
<tr>
<td>“extreme adsorption”</td>
<td>high enthalpy, increased SSA, equilibrated initial methane, no source, no decay</td>
<td>study effects of extreme adsorption</td>
</tr>
<tr>
<td>“spike”</td>
<td>high enthalpy, no initial methane, 24h source at Gale Crater, no decay</td>
<td>study effect of adsorption on dispersion after emission</td>
</tr>
<tr>
<td>“spike without adsorption”</td>
<td>no adsorption, no initial methane, 24h source at Gale Crater, no decay</td>
<td>reference for “spike”</td>
</tr>
<tr>
<td>“fast decay”</td>
<td>high enthalpy, no initial methane, constant source at Gale Crater, 1 day decay</td>
<td>study effect of adsorption and fast destruction on mixing</td>
</tr>
<tr>
<td>“fast decay without adsorption”</td>
<td>high enthalpy, no initial methane, constant source at Gale Crater, 1 day decay</td>
<td>reference for “fast decay”</td>
</tr>
</tbody>
</table>
2.3 Water

Here I describe the subsurface model for water. I also discuss the treatment of thermal conductivity in the soil, how the ice content in the subsurface is limited, and how a good initial state can be found.

2.3.1 Soil Description

Like the model for methane, the subsurface model for water simulates diffusion and adsorption, but adds the possibility of condensation and sublimation of water ice. It is also purely diffusive. The boundary condition at the surface is still free exchange with the atmosphere as long as there is no ice of any kind. If there is water ice, the water saturation pressure is assumed at the boundary. If there is only CO$_2$ ice no water can enter the soil, but the soil can still emplace water ice at the surface, if the conditions allow it.

In order to improve the depth resolution of the potential ice table, the number of subsurface layers is increased to 55, following a more complex profile designed to increase the resolution for all layers while still increasing the layer thickness with depth. The maximum depth is kept similar to about 25 meters. Even though the lower layers had been found to be too deep to impact the atmosphere in any significant way in the methane simulations, the deep layers are important for modelling the seasonal temperature variations correctly. The depths for each layer as well as the used formula can be found in Table 3 in the appendix.

Just like in the methane simulation water ice filling the pores slows down diffusion, but here it also impacts the diffusion by influencing the amount of water vapour. The model ensures that the amount of water vapour stays at the saturation pressure whenever water ice is present in a subsurface layer.

A simplified adsorption isotherm is used. The adsorbed water is proportional to the partial pressure, but adsorbs no additional water once the amount of one monolayer (a layer one molecule thick) has been reached.

The adsorption enthalpy and specific surface area are free parameters for water
as well, but only one set of values is used. For the specific surface area the same default value is the as for methane with 17 m$^2$/g. For the enthalpy of adsorption a value of 21 kJ/mol is used, based on measurements by the Curiosity rover (Savijärvi et al., 2016).

Like for the methane simulations some assumptions have been made, due to the lack of knowledge or difficulty of implementation. While the first four assumptions from Section 2.2.1 still hold true, there are some additional assumptions made:

- When both water and CO$_2$ ice are present on the surface, they are treated as always well mixed. They are both in exchange with the atmosphere and the water ice is able to exchange with the subsurface.

- The geothermal gradient can be neglected.

### 2.3.2 Thermal Conductivity and Ice Table Depth

The depth at which ice is stable is dependent on the thermal conductivity of the soil, since the saturation pressure depends exponentially on the soil temperature. The treatment of thermal conductivity therefore requires some special consideration.

In reality the presence of water ice raises the overall thermal conductivity of the soil, both because it increases the contact area between the soil grains and because its thermal conductivity is higher than that of the soil. It is expected that this raises the ice table compared to a constant thermal conductivity, since temperature variations are lower in layers with high thermal conductivity (Schorghofer, 2010). However, modelling this is outside the scope of this work, since the simulation timescales are greatly increased by slow changes that would be caused by this feedback mechanism.

There are three scenarios for the thermal conductivity used in this work:

1. The thermal conductivity can be set to different values depending on the depth. In the current version of the model without any subsurface ice, thermal conductivity is constant with depth except near the poles,
where water ice can be expected in the soil. There, the upper layers have a low thermal conductivity as measured from orbit. The deeper layers have a higher thermal conductivity which is also constant with depth and in each hemisphere. The depth and value of the thermal conductivity have been optimized to reproduce the observed amounts of CO$_2$ ice on the surface and are not based on direct observations. The shallow and deep maps of thermal inertia (which is proportional to the square root of thermal conductivity) for this scenario can be seen in Figure 5.

2. The thermal conductivity can be set to a high value (assuming the presence of ice) at all depths for gridpoints where subsurface ice is expected. This is done by taking the thermal conductivity of the *deepest* layer from the default configuration and imposing his value for all layers of the respective gridpoint. This corresponds to Figure 5b.

3. The thermal conductivity can be set to a low value, equal to the one measured from orbit at the surface for all depths. This is done by taking the thermal conductivity of the *shallowest* layer from the default configuration and imposing his value for all layers of the respective gridpoint. This corresponds to Figure 5a.

Each scenario has its advantages and disadvantages. Scenario 1 is the one used in the reference simulations, which means its the only one where the effect on
the water cycle can be meaningfully evaluated. The downside is that it has basically a predefined ice table, since the ice is expected to be more stable in the high thermal conductivity layers. Since the depth of the transition is only based on the amounts of surface CO$_2$ ice, this likely leads to unrealistic ice table depths.

Scenario 2 can be used to evaluate if a soil with a lot of ice is possible, but it is very unlikely to be realistic.

Scenario 3 should give a good estimate of realistic ice table depths, even though they are likely still to deep due to the missing feedback on thermal conductivity. The results can also not be compared to the reference simulations.

2.3.3 Limiting the Ice Content

For simulating reality as close as possible, it is desirable to limit the ice content of the soil to a certain fraction of available pore space. Once this fraction is reached, there are no pathways left for transport processes and no additional ice can be deposited. In this work this fraction is arbitrarily chosen to be 80%. Implementing this, however, comes with some difficulties. The default approach is to reduce the diffusion coefficient inside the ice filled layer, to significantly slow down or stop diffusion. This approach proves ineffective and causes an instability that is discussed in Section 3.2.3. The underlying problem is that the crucial diffusion coefficient is not the one within the layers, but the one at the interface between the layers which has to be interpolated.

To solve this problem a different approach is implemented. The interpolation is replaced with taking the lower ice content of the two layers as the interface value. To limit the ice content, the possibility to “close” interfaces is introduced. Once an ice layer reaches saturation, the fluxes at the top and bottom interface are checked. If the flux at an interface points into the saturated layer, the interface is “closed” by lowering the diffusion coefficient at that interface to $10^{-6}$ times the ice free value. Slowing down the diffusion by this much is sufficient to limit the ice content to the saturation value and has another significant advantage. Because the flux is not zero, it’s sign can be evaluated and the interface can be “reopened” when the flux is pointing out of the layer.
2.3.4 Initialization and Decoupled Subsurface Model

Finding a good initial state is quite difficult for water, since the water ice is expected to have complex profiles (Schorghofer and Aharonson, 2005) and no detailed observational data is available. I therefore decided to initialize the soil as completely dry. There is a severe drawback to this approach: the subsurface is able to hold very large amounts of water compared to the atmosphere and diffusion is a relatively slow process. Therefore, the formation timescale of subsurface ice is very long. Furthermore, it is very likely that, in the beginning, the soil uptake capability exceeds the capability of the atmosphere to supply water, which would artificially dry out the atmosphere and slow down the emplacement process even further. Running the full atmospheric model for hundreds of martian years is, however, prohibitively expensive computationally. Even on the fastest available machine, the IRAP Titan cluster, the model simulates only about three Martian years in 24 hours.

To solve this problem I, together with Ehouarn Millour from the LMD, developed a subsurface model that runs decoupled from the atmospheric simulation, called noGCM. The idea behind this is that the current atmospheric model reproduces the observations relatively well and the subsurface should therefore be in a steady state with that atmospheric model.

In this decoupled model all atmospheric dynamics and physical processes are switched off and only the subsurface model is run as usual. Since no useful boundary condition can be provided by the atmospheric model any more, the required data is read from a file. The data in this file is computed beforehand from a full atmospheric model without water in the subsurface. This also means that there is no feedback from the soil to the boundary conditions. Compared to the full model, the decoupled model loses the ability to run in parallel. Nevertheless, the decoupled model can run about 100 Martian years in 24 hours with these changes and a reduced spatial resolution or 25 martian years in full resolution. A increased timestep of 1 hour is used to speed up the simulation. After one hundred martian years, the resulting state can then be used to initialize the soil for the full atmospheric simulation.

The results from the decoupled model can also be used by themselves to study
the behaviour of water in the subsurface. For example ice table depths, adsorbed water content, and total water content can be compared to measurements.

In order to check if the model behaves as expected, I predict the ice table depth by comparing the average surface water vapour abundance to the average saturation vapour pressure in the soil layers. In equilibrium and on average, the water vapour in all the soil layers should reach the average surface water vapour abundance. If this abundance is above the saturation pressure in a layer, ice is expected to form in this layer. Due to the exponential dependence of the saturation pressure on temperature, the layers near the surface with higher temperature variations have a higher average saturation pressure. This is illustrated in Figure 6. However, this is only an estimate, since all dynamical processes which could have an influence on the ice are averaged out.

**Figure 6:** Example illustration of the ice table depth prediction. In blue the local yearly average of the water saturation pressure, in green the average value at the surface. The ice table is predicted to be where the two lines intersect.
2.4 Computing Infrastructure

Since many of the simulations are limited by computing power, and the available infrastructure changed significantly over the course of this work, I present it here.

For all the methane simulations I use the IRAP server Hyperion, powered by an Intel Xenon E5420 @ 2.50GHz. Both the hard and software on it are about ten years old. This made it impossible to run the updated version of the model, because of compilation problems.

To run tests for the water simulations I use my laptop, powered by an i7-6500U @ 2.5GHz. It is about 55% faster than Hyperion, but has the disadvantage that it can’t run continuously.

I tried running the water simulations on the IRAP server Hyperion 2, powered by an Intel Xenon E5-2609 v2 @ 2.50GHz. It is about 25% faster per core than Hyperion, but is unable to run the new model in parallel, because of its old software. It was therefore too slow to be of any use.

For the noGCM simulations I used the office computer of Ehouarn Millour from the LMD, powered by an i5-4690 CPU @ 3.50GHz. It has the fastest single core performance available to me, with about 110% faster than Hyperion.

The full water simulations are run on the IRAP computing cluster Titan. The used node is powered by two CPU E5-2650 v3 @ 2.30GHz. It has up to date software and can run the simulation on 24 cores, resulting in a speed increase of about 1200% over Hyperion.
3 Results and Discussion

I will first go over the results for methane, followed by the results for water.

3.1 Methane

This subsection covers the effect of the subsurface on the global methane cycle and the specific situation at Gale Crater. I present the results of the spike emission simulation as well as the fast decay and clean regolith simulations.

3.1.1 Global Cycle

Due to the difficulties of initializing the methane in areas that get covered by CO₂ ice in the winter, it takes about seven Martian years for the high enthalpy simulation to get close to a repeatable cycle. In the initial years the polar regions release a large amount of methane in the summer, but take up very little in the winter, because then they are mostly covered by ice. The overall amount of methane in the atmosphere therefore increases dramatically and is then far above the equilibrium value for all the other regions. After loosing all their excess methane the polar regions reach an equilibrium and the upper layers on the rest of the planet also reach equilibrium after adsorbing some of the additional atmospheric methane. What remains is a slow decrease in total atmospheric methane as the deep layers outside the polar regions adapt. This slow uptake has no influence on the seasonal cycle.

Increasing the enthalpy of adsorption from the previously used value of 18 kJ/mol to 31.5 kJ/mol has very strong effects. As can be seen in Figure 7 the variations over one Martian year change from barely visible to almost 15% on a global level.

The high enthalpy curve is in Figure 7 is highly asymmetric. While it hardly reaches less than 3% below the average in the first half of the year, it peaks to almost 9% above the average in the second half. This is caused by the current orbit of Mars with an eccentricity of about 0.1 and the resulting temperature differences between the hemispheres. Mars is closest to the Sun during the
Figure 7: Total amount of atmospheric methane normalized to the average over the course of one Martian year for simulations with an adsorption enthalpy of 31.5 kJ/mol and with an adsorption enthalpy of 18 kJ/mol. Both use a SSA of 17 m²g⁻¹. While there is almost no variation for low enthalpy, the variations reach almost 15% for high enthalpy.

southern summer and northern winter. Because of this, the southern hemisphere has warmer summers and cooler winters compared to the north, which translates to a larger variation in the adsorbed methane content.

During the first half of the year, the uptake of methane in the southern winter outweighs the release in the northern summer. Then, in the second half of the year the southern summer causes the large peak between 250 and 300 degrees solar longitude. It is important to note that the uptake and release of methane always happens at the same time on the two hemispheres in their respective winter and summer. Therefore, the change in global methane only shows the imbalance between the hemispheres.

The main contribution to the variations comes from the high latitudes, which can be seen when looking at the fluxes in Figure 8a. This is not surprising, since adsorption is a highly temperature dependent process and most effective at cold temperatures (see Equation 1).
(a) Methane flux into the soil per unit area normalized to its maximum. Largest fluxes around ±50° latitude.

(b) Variations in the exchange between atmosphere and subsurface due to CO₂ ice on the surface.

Figure 8: Longitude averaged fluxes and exchange variations over one Martian year for the high enthalpy simulation.

Interestingly, the latitudes around 40 to 50 degree north and south contribute much more than latitudes closer to the poles, even though those are colder. There are two different reasons for this.

1. Areas closer to the pole get covered by the seasonal CO₂ ice cap during the winter, which prevents any exchange with the atmosphere. This can be seen in Figure 8b. The short time window between reaching a temperature low enough for additional adsorption and ice coverage means that only small amounts of methane are taken up by the soil. As temperatures rise during the summer, the soil is free to exchange with the atmosphere, but not much methane is available for release.

2. The very high latitude areas have a very shallow water ice table. This prevents the methane from penetrating deeper into the soil and therefore reduces the uptake and release capabilities.

Figure 8a also shows stronger fluxes per unit area in the north than in the south, even though this is not reflected in the global values (see Figure 7). The reason for this is that the important latitude bands for adsorption are further away from the pole in the southern hemisphere and the larger area leads to an overall greater influence even with smaller fluxes per unit area.
This asymmetry in the important latitude bands is caused by the difference in temperature variation due to the eccentricity of the orbit. The southern winter is colder than the northern one, causing the CO$_2$ ice cap to extend further towards the equator and inhibiting exchange between soil and atmosphere.

Figure 9: Comparison of longitude averaged methane column densities over one Martian year. The data has been normalized to its average value.

The methane released and taken up strongly influences the global distribution of methane. Even without any adsorption there are variations in methane column density over the course of the martian year, which can be seen in Figure 9a. This is caused by the sublimation and condensation of CO$_2$ on the surface. Condensation leaves the non-condensible gases like methane behind and concentrates them, while sublimation dilutes the non-condensible gases. In Figure 9a the peaks of methane over the winter poles and lows of methane during spring and summer can be clearly seen.

When comparing this reference simulation with the high enthalpy simulation in Figure 9b multiple interesting effects are visible:

- The peaks above the winter poles are weaker, because they coincide with times of uptake in their respective hemispheres.
- The lows in springtime above the poles are also weakened, because they coincide with times of release in their respective hemispheres.
• There are additional peaks at high latitudes in the respective summers, caused by the continued release of methane in the warm season.

• Regions of high methane content spread south from the northern summer peak. These are caused by the transport of methane by the global circulation.

• The southern peak does not experience a similar transport phenomena. This is due to the great differences in global circulation patterns between the northern and southern summer.

3.1.2 Seasonal Cycle at Gale Crater

Comparing the results of the simulation with the extreme adsorption (high SSA, high enthalpy) with the reference without adsorption in Figure 10 clearly shows the strong effect adsorption has on the methane concentration at Gale Crater. While the no adsorption case follows a thin line with only small variations, the extreme adsorption case forms a thick band due to the diurnal (daily) cycle and shows strong seasonal variations. The methane concentration falls in the beginning of the year, then starts rising around the beginning of the northern summer at 90° solar longitude and peaks around the beginning of northern fall at 180° solar longitude. After a small decline following the peak, it stays roughly constant for the rest of the year. The strength of the diurnal cycle varies over the course of a year and has its maximum between 50 and 100 degree solar longitude.

Overall, the local contribution to the seasonal cycle is small, which can be seen in Figures 8a and 9b. The biggest contribution is the transport of methane from the higher latitudes to Gale Crater. This is especially visible between the 150 and 200 degree solar longitude, when comparing Figure 10 and 9b. One can see that the peak in methane at Gale Crater is caused be the transport of methane from the northern high latitudes.

Compared with the measurements by Curiosity at Gale Crater the extreme adsorption simulation shows a similar profile and a similar amplitude of the variations in methane concentration. Only three measurements have error bars
Figure 10: Volume mixing ratio variations at Gale Crater over one Martian year. The extreme adsorption simulation in green is compared to no adsorption in blue and the measurements by Curiosity in red. Gaps in the green band are caused by the temporal resolution of the simulation output and have no physical meaning.

which are completely outside of the simulated concentrations and of those two are very close. Adsorption could therefore be a possible process to explain the measured seasonal variations. A local source is not required.

3.1.3 Diurnal Cycle at Gale Crater

While the local uptake and release of methane has a small effect on the average mixing ratio at Gale Crater, it does shape the diurnal cycle. In Figure 11 a high uptake and a high release situation are shown over the course of one sol. The cycle is very similar from one day to the other, but shows seasonal variations. The flux curve follows a relatively similar shape in both Figure 11b and 11a, but are offset from each other. They are both driven by the diurnal temperature variations. Starting with the sunrise around six o’clock
local time the surface temperature starts to rise and reaches its maximum in the afternoon. The flux follows with some lag, since the change in surface temperature needs to be conducted into the soil to have an effect on the adsorption. In both cases the flux out of the soil reaches its maximum shortly before sunset around 18 o’clock.

This release of methane has, however, only a small effect on the surface mixing ratio during the day. This is because during the day the surface heats up faster than the atmosphere and drives very efficient turbulent mixing between the atmospheric layers. Therefore, any methane released or taken up is quickly diluted or replaced.

This picture changes after sunset. Since the surface now cools faster than the atmosphere a very stable stratification develops. The only means of transport between the layer close to the surface and the rest of the atmosphere is now relatively slow diffusion. In Figure 11a, showing the high release situation, a sharp rise in the surface mixing ratio can be seen after sunset, which is driven by the continued release of methane from the soil. It reaches a peak when the flux comes close to zero around midnight and starts to fall to below the daytime value as temperatures continue to fall. In Figure 11b the peak

Figure 11: Diurnal cycle of the local flux and the surface mixing ratio of methane during times of release and uptake. Flux out of the soil normalized to its maximum in green and surface mixing ratio normalized to its average in blue. Zero flux marked as dashed line.
is much smaller and earlier as the flux reaches negative values much quicker. The atmospheric surface layer is then continually depleted of methane until it is replenished during the next day.

3.1.4 Spike Simulation

The spike simulation shows that methane is mixed relatively evenly around the planet in less than 40 days. This is illustrated in Figure 12. Adsorption is not able to contain the methane in one region, because it is too slow. When compared to the reference spike simulation without adsorption, the change in methane distribution is negligibly small. If there is adsorption, the total amount of methane in the atmosphere slowly decreases with time. But even with strong adsorption and a initially “clean” regolith only a small fraction of methane is adsorbed during the global mixing time. Therefore any methane detected by Curiosity should still be detectable by TGO around the globe in this scenario. Adsorption alone cannot explain the conflicting data of TGO and Curiosity.

**Figure 12:** Methane column density normalized to the maximum value 2, 10, and 40 sols after a 24 hour emission event at Gale Crater. After 40 sols the methane is very uniformly distributed over the whole planet. Mars map shown in dark grey.
3.1.5 Fast Decay Simulations

The fast decay simulation shows that methane can be somewhat confined around its source region, if there is a very fast destruction process present. Figure 13 shows the distribution for a source at Gale Crater with a one day decay timescale. Even with such a fast decay, the area that reaches more than $10^{-3}$ of the maximum concentration is about 60° in latitude and 100° in longitude. Due to the low number of TGO measurements close to the equator, there is only one of them in this region and it is on the very edge. Therefore a very fast destruction process could explain the conflicting data of TGO and Curiosity. The possible nature of such a process, however, is unknown.

**Figure 13:** Methane column density averaged over one year and normalized to the maximum value for a continuous source at Gale Crater and a one day decay. The locations of the TGO measurements are marked with green stars. Mars map shown in grey.

When comparing the fast decay simulations with and without adsorption, there is almost no difference. Since methane is destroyed and replaced so
quickly, the uptake of the soil has almost no influence on the amount of atmospheric methane. Just like for the spike simulations the adsorption is too slow to have an impact on the distribution of methane. This also means that the fast decay makes any seasonal cycle that was present in the other simulations impossible. This makes it hard to explain the conflicting data from TGO and Curiosity and the seasonal cycle at the same time.

3.1.6 Clean Regolith

When a “clean” regolith is combined with a methane-rich atmosphere, the atmospheric methane gets adsorbed relatively quickly in the beginning. It drops to half its initial value after about 150 sols and reaches one third after about a year. After the first year the beginning of a seasonal cycle can be observed and the atmospheric methane decreases much more slowly. To reach two thirds of the methane content at the one year mark, another two years are needed.

The regolith can therefore be a quick and effective buffer for spikes in atmospheric methane by greatly reducing the atmospheric methane content on a timescale of about one year. This can, however, only work if methane can be removed again from the soil before the next event. This could happen through slow release from the soil and subsequent photodissociation or potential chemical processes in the soil.
3.2 Water

This subsection covers the distribution of ice and the ice table in the noGCM simulation, as well as the ice profile and formation mechanism. I also discuss the effect of adsorption and the influence of the subsurface onto the atmospheric water cycle.

3.2.1 Ice Distribution

After running the noGCM code for 100 Martian years a considerable amount of permanent ice has been emplaced in the subsurface. This can be seen in Figure 14, which shows the ice distribution for the homogeneous low thermal conductivity scenario and the inhomogeneous thermal conductivity scenario. The missing ice at some very high northern latitude grid points is not physical. Instead these are the gridpoints where the permanent water ice of the north polar cap is modelled and the subsurface is not simulated. In the inhomogeneous scenario more ice has been deposited, especially in the north. This is due to the stabilizing effect the high thermal conductivity in the deeper layers provides.

When comparing the maximum ice over the year in Figure 14a and 14b to the minimum ice over the year in Figure 14c and 14d it is clear that there is a lot of seasonal ice. It is reaching to much lower latitudes than the permanent ice and gets deposited in the respective winter, but is not stable enough to persist in the summer.

The minimum ice is more or less where it is predicted by the comparison between the average vapour pressure at the surface and the saturation vapour pressure in the soil, seen in Figure 14e and 14f. There are almost no differences in the location of the predicted ice stability. There are some gridpoints, especially in the northern hemisphere around 100° east, where ice is stable even though it was predicted to be unstable. The reason for this unexpected ice is likely caused by the dynamics in the subsurface, which are not captured by the simple comparison of average vapour pressure. The speed of the diffusion changes with temperature, and there is a lot of water vapour available.
Figure 14: Subsurface ice column distribution over the last year of two 100 year noGCM simulations and prediction of ice stability. Mars map shown in grey.
during the northern summer. This vapour can enter the soil quickly during the summer, but only part of it can leave again during the winter, because the diffusion has become much slower.

3.2.2 Ice Table

While the different thermal conductivities had little effect on which gridpoints had stable subsurface ice, there is a large effect on the depth of the ice table. The depth distributions of the permanent ice table for the homogeneous low and inhomogeneous thermal conductivity scenarios are shown in Figure 15.

Figure 15: Ice table depth for the homogeneous low and inhomogeneous thermal conductivity scenario. Mars map shown in grey.

In the homogeneous scenario (Figure 15a) the ice table qualitatively behaves as expected, becoming deeper the further away from the pole a gridpoint is. In the inhomogeneous scenario (Figure 15b) this is not the case and the strong influence of the high thermal conductivity layers is clear. Wherever the thermal conductivity is high in the deeper layers, the ice table is much shallower than in the inhomogeneous case. The ice gets stabilized at the transition from low to high thermal conductivity which is rather shallow.

The ice table depths are compared to the observations and predictions for the three thermal conductivity scenarios in Figure 16. In the homogeneous low
(a) Homogeneous low thermal conductivity scenario.

(b) Inhomogeneous thermal conductivity scenario.

(c) Homogeneous high thermal conductivity scenario.

(d) Comparison to prediction. Scenarios colour-coded corresponding to Figures 16a, 16b, and 16c.

Figure 16: Comparison between the ice table depths from the simulations with the ones measured by Mars Odyssey and the ones predicted. The dashed lines mark equal depth.

In the homogeneous low thermal conductivity scenario the ice table is generally too low compared to the observations, while it is actually too shallow for a few gridpoints. This is not really surprising for two reasons. On the one hand in many of the gridpoints the ice content has not reached saturation yet and the ice table starts rising after saturation has been reached. This is discussed in more detail in Section 3.2.3, but running the simulation until an equilibrium has been reached is computationally unreasonably expensive. On the other hand the neglected thermal feedback of the ice would raise the ice table as well.

This can be seen very well in Figure 16b, where the inhomogeneous scenario
is compared to the observation. For the gridpoints with high thermal conductivity layers the ice table is much shallower and is now actually too shallow. The gridpoints with very deep ice tables remain unchanged, since these are at lower latitudes and have the same thermal conductivity in both scenarios.

Having the high thermal conductivity in all layers has the opposite effect, which can be seen in Figure 16c. In this case the thermal variations from the surface penetrate much deeper into the soil and push the zones with stable ice downward. The ice table is therefore even deeper than in the homogeneous low thermal conductivity scenario.

It is important to note that the observations from Mars Odyssey are only able to detect water in the upper few decimetres of the soil. A deep ice table, as in some of the simulated gridpoints, would therefore not actually be found.

Comparing the simulations to the prediction in Figure 16d shows that the prediction does not give a very good estimate for all three scenarios. Most points are close to the line of equal depth, but they do have a very large spread, especially considering that Figure 16d uses logarithmic scales. It is also important to note that not all gridpoints are shown, but only those who have ice predicted and actually occurring in the simulation.

### 3.2.3 Ice Profile and Formation

Stable subsurface ice has a typical depth profile that can be seen in Figure 17a. There is a very sharp jump at the top of the ice layer, rising from no ice or almost no ice to the maximum ice density. Over time the amount of subsurface ice increases in every layer with stable ice as long as it doesn’t come close to saturating the pore space, which is also visible in Figure 17a.

When the ice content reaches close to saturation in the peak layer, the initial approach of just reducing the diffusion coefficient inside the saturated layer develops an instability than can be seen in Figure 17b. The ice content in the peak layer actually continues to rise to non-physical amounts and the ice below the peak layer develops a saw tooth profile that spreads downwards as time goes on.

This is a direct consequence of the interpolation and the shape of the ice
(a) Typical ice profile with depth for stable subsurface ice. A strong peak is followed by a quick decline in ice content with depth.

(b) Ice profile with instability which develops with the default approach, when the ice saturation fraction reaches close to one. With time the instability spreads downwards.

Figure 17: Ice profiles from the noGCM simulation.

profile. The saturated layer has a diffusion coefficient of almost zero, but since the layer above has almost no ice, the interface between the layers is still able to carry water into the saturated layer. On the other side the layer below the saturated layer actually starts to loose ice. This is because its supply of water from above is reduced, but the layers further down still have much less ice and still take up a similar amount of water. Since the general direction of diffusion is downward, more water is removed from the layer than refilled from the top. A new peak develops two layers below the initial saturation. Once this new peak reaches close to the saturation value, the cycle repeats and the instability spreads downwards.

The new implementation of closing interfaces and replacing the interpolation with a minimum does solve this problem. It limits the ice to the saturation value and removes the instability. This can be seen in Figure 18.

The new implementation also shows another effect. Once the ice reaches saturation in the peak layer, the layer above starts filling with ice, thereby raising the ice table. This continues for a few layers until an equilibrium is reached. During the time frame of the simulation only very few gridpoints reach saturation and show this effect. However, a test with rescaled ice profiles showed that all gridpoints with stable subsurface ice show this behaviour.
In the gridpoints with stable subsurface ice, the ice layers do not grow continuously. Instead, there is a pulse of additional ice once a year. The responsible process can be seen in Figure 19. During the winter, ice is stable in all layers at the gridpoints with stable subsurface ice. During the spring and summer the surface gets heated and the seasonal thermal wave starts to travel into the soil. As the upper soil layers get warmer, the ice above the stable ice layer sublimates, which can be seen in Figure 19a. The resulting excess water vapour diffuses in both directions, partly upward into the atmosphere and partly downward towards colder layers, where it can condense again. This can be seen in Figure 19b. At the stable ice layer the wave has lost most of its strength and is unable to sublimate the ice completely. More ice is deposited than lost every year, causing it to build up. Nevertheless, the thermal wave continues to travel through the ice layer and sublimates part of the ice, causing a general downward flux into deeper layers. As the temperature variations get smaller with depth the flux also decreases, giving rise to the ice profile seen in Figure 17a. At the end of summer, the surface temperatures decrease again and the soil can take up water from the atmosphere, reforming the ice in the shallower layers.
(a) Subsurface ice density. Ice gets pushed by thermal wave into the stable ice layer.

(b) Subsurface interlayer fluxes. Downward fluxes in front of the thermal wave and upward fluxes behind.

Figure 19: Subsurface ice gets pushed by the seasonal thermal wave

3.2.4 Adsorption

The enthalpy of adsorption of 21 kJ/mol used in the simulation is much lower than the enthalpy of condensation under the conditions on Mars of roughly 50 kJ/mol. Therefore adsorption only plays a minor role whenever the relative humidity gets high enough to form water ice. Since adsorption gets favoured by the same conditions as ice formation, storage of water in the soil becomes a two stage process. As conditions get colder and wetter, adsorption starts to increase, up to the point of ice condensation. From there on ice takes over as the primary form of water storage. This means that in the high latitude regions adsorption only plays a significant role in the summer months, when the ice in the upper layers has become unstable.

To determine if the low latitude hydrogen measured by Mars Odyssey could be explained by adsorbed water, the map of the adsorbed subsurface water is compared to the map of the measurements in Figure 20. In the high latitude regions there is almost no adsorption due to the dominance of ice, but the same ice can explain the high measurements in these regions. Looking at the low latitude regions the patterns are very different. Many regions show high water content in the simulation and low hydrogen content in the observations. Therefore adsorption alone is unable to explain the distribution of water.
equivalent hydrogen in most of these regions with the current parameters. It is also unlikely that any change in adsorption strength will significantly change these patterns, because it would primarily change the amount of adsorbed water not its distribution.

### 3.2.5 Influence on the Water Cycle

Initializing the soil in a full atmospheric simulation with the results from the noGCM simulation with inhomogeneous thermal conductivity produces a repeatable water cycle after a few Martian years. However, this water cycle is generally wetter than the reference water cycle, which can be seen in figure 21. The shape of the curve is similar to the reference simulation, but offset to a higher average.

A more detailed comparison can be done with the longitude averaged plots in Figure 22. The averaged observational data from the Thermal Emission Spectrometer on board Mars Global Surveyor can be seen in Figure 22a. It is relatively similar to the reference simulation in Figure 22b, but some aspects are not properly represented in the simulation. For example the peak in the northern summer is too strong in the simulation and the area of high water vapour in the northern hemisphere during the southern summer is not properly reproduced.
Figure 21: Globally averaged water vapour in the atmosphere for the reference and the new water cycle. The new cycle is generally wetter, but has a similar shape.

When comparing the water cycle of the new simulation with a subsurface in Figure 22c to the reference simulation, it is again clear that the new water cycle is too wet. The water vapour levels are elevated everywhere, except over the polar caps during the respective winters where almost all the water freezes at the surface. Two areas stand out with the biggest changes: the northern and southern summer peaks. In the north, the peak reaches about the same maximum values (not visible in the figure), but extends further in latitude. It also reaches high amounts of water vapour earlier in the year. In the south the situation is different. The peak has about the same extend in latitude and time as the reference case, but the maximum water vapour density is about twice as high.

The reason for the regional differences can be found by examining the longitude averaged flux in Figure 23. The plot has been adjusted for the different area of the latitude bands and shows the amount of flux per degree latitude. It can be seen, that while there is some flux all over the globe, the regions with the highest flux in and out of the soil are the polar regions. As the CO$_2$ ice sheets retreat and reform, large amounts of water are taken up by the soil. It is then released again during the respective summers, causing the increased peaks over the poles. Overall the subsurface releases more water than it is taking up, even after a few Martian years.
Figure 22: Comparison between the new and reference water cycles.
While the exact underlying reasons for these changes in the new water cycle are not known, there are different hypotheses:

1. In a test simulation, where the homogeneous high thermal conductivity noGCM simulation was used for initialization, the water cycle stayed very close to the reference with only temporary differences. Since that simulation had a much deeper ice table, it might be that the ice table is too shallow, interacting too quickly with the atmosphere. A solution could be to simulate the thermal properties of the soil more realistically, including thermal feedback from the ice. This would require a significant amount of work and testing.

2. Due to the shallow ice table, the feedback of the subsurface onto the surface and atmospheric conditions might be too strong to neglect. Neglecting this feedback is one of the central assumptions that makes the noGCM initialization possible. If this is indeed the case, the noGCM approach is fundamentally flawed.

3. There might be an issue with the timestep used. The noGCM simulation uses a timestep that is four times longer than the full atmospheric simulation for performance reasons. The data for the boundary conditions is also not averaged but supersampled. If this is the problem, it would be easy to fix, but increase computational cost significantly.
4 Conclusion and Future Work

For methane, the simulations have shown that adsorption can potentially be the reason for the observed seasonal variations. A comparison with the one dimensional results from Moores et al. (2019) shows a similar seasonal curve, but the underlying reason is different. In the 3D simulation in this work the variations are caused by the adsorption at high latitudes and transport towards the equator, while local adsorption combined with a source causes the variations in the 1D simulation from Moores et al. (2019).

However, the match of the simulation with the observations is not perfect. In the future additional source and destruction scenarios can be tested to better explain the observations. These could be a global flux from sources deeper in the crust, or sources in specific areas. Destruction scenarios could include destruction in the soil or on dust particles.

The simulations have shown that adsorption cannot explain the conflict between the data from Curiosity and TGO. Only extreme scenarios with a very efficient destruction process could possibly resolve the conflict. The nature of such a process is unknown and its existence therefore unlikely.

In general more observational data is needed to determine the role of adsorption for methane. Future high precision measurements by Curiosity over the course of a day could determine the local strength of the adsorption process, since strong adsorption causes a distinct diurnal cycle. The methane model can also be improved in the future by switching to the same newer GCM version that is used for water. This would improve temperature accuracy, soil resolution, and simulation speed. It would also make it possible to run water and methane in the same model and simulate the effect of dynamic water ice on methane adsorption.

For water, the simulation mostly produces the expected ice distributions and profiles. However, compared to observations the ice table depths do not match very well. This is either caused by inaccuracies in the simulation or by the ice being out of equilibrium, with the first one likely having the bigger influence. To improve this a more refined treatment of the soils thermal properties is necessary that includes ice feedback on thermal properties. Longer noGCM
simulation times could be achieved through palletization and could improve the results as well, especially when thermal feedback is implemented. Vertical profiles for very high ice contents can be correctly simulated, after an instability was overcome. Improvements in the details of the diffusion calculation in high ice content layers can still be made, but are not expected to have a large impact.

With the used parameters adsorption only plays a minor role, since ice formation is favoured at low temperatures. Adsorption is also not able to explain the water-equivalent hydrogen observed in the soil at low latitudes. In the future, other values for the enthalpy of adsorption and their effect could be studied. Values higher than the enthalpy of ice formation require the implementation of a more sophisticated and more realistic isotherm.

The new way of initializing the subsurface using a decoupled subsurface model has proven partly successful. With this initialization a full atmospheric simulation including the subsurface could be run, without completely disrupting the water cycle. However, the atmosphere is too wet compared to the reference simulation and observations. In the future possible reasons for this mismatch should be investigated, including missing thermal feedback, subsurface feedback onto surface conditions, and timestep length.

There are still many ways to improve the model overall in the future. But a lot of its important parameters currently suffer from a lack of comprehensive and reliable data. Continued measurement by current mission and possible future missions will possibly be able to fill some of these gaps.

Early results for both methane and water were submitted to the 9th Mars Conference in two abstracts. They were written together with Pierre-Yves Meslin and can be found in the appendix.
References


Appendix

This appendix contains the exact layer depths of the methane and water models in Tables 2 and 3 on Pages 56 and 57. They are followed by the two conference abstracts submitted to the 9th Mars Conference.

**Table 2:** Methane model soil layer depths. Values are given as the mid-layer depths and rounded to two decimals. The depth for the layer number \( n \) in meters is:

\[
d(n) = 2 \cdot 10^{-4} \cdot 2^{n-0.5}
\]

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Table 3: Water model soil layer depths. Values are given as the rounded mid-layer depths. The depth for the layer number n+1 in meters is:

\[ d(n + 1) = 2 \cdot 10^{-4} \cdot n^{2.9} \times (1 - \exp(-n/20)) + 2 \cdot 10^{-4} \]

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Implications of a Strong Adsorption Process on the Variability of Methane in the Martian Atmosphere. P.-Y. Meslin¹, J. Weinmann¹, J. Moores², C.L. Smith³, F. Forget⁴, E. Millour⁵, R. Gough⁶, S. Atreya⁶, C. Webster⁷, P. Mahaffy⁸, ¹IRAP, UPS-CNRS, Toulouse (meslin at irap.omp.eu), ²York University, Canada, ³Australian National University, Australia, ⁴Laboratoire de Météorologie Dynamique, Paris. ⁵University of Colorado, Boulder, CO, ⁶University of Michigan, Ann Arbor, MI, ⁷NASA-Jet Propulsion Laboratory, Pasadena, CA, ⁸NASA-Goddard Spaceflight Center, Greenbelt, MD.

Introduction: The difficulty to understand the martian atmospheric methane cycle originates from the difficulty to constrain its production mechanism(s) and to account for the differences seen by several instruments [1-9], whose observations appear to be inconsistent with each other and with our current understanding of the loss mechanisms of methane in the martian atmosphere [10]. Very strong constraints have been provided by the detections of sporadic spikes of methane at different locations on Mars [1-8] and by the lack of any methane detection by the Trace Gas Orbiter (TGO) from April to August 2018, with an unprecedented level of sensitivity [9].

In addition to the reports of intermittent methane spikes, the Tunable Laser Spectrometer (TLS), part of Curiosity’s Sample Analysis on Mars (SAM) suite, also recorded seasonal variations of methane (around a mean value of 0.41 ppbv) [11], whose amplitude is stronger than currently predicted by GCM models and whose origin thus also remains to be explained.

If they can ever be reconciled, all these observations indicate that little is understood about both the origin, release mechanism and destruction or temporary storage of methane in the (regolith + atmosphere) environment. New processes must therefore be explored and tested.

Methane adsorption as a potential source of variability: Adsorption of methane in the regolith, which is a temperature-dependent and reversible process, was suggested to be responsible for a possible atmospheric seasonal cycle, based on experimental measurements of its characteristic enthalpy ($\Delta H_{ads}$ ~18 kJ mol$^{-1}$) [12]. This process has the advantage of inducing time and space variations without the need for additional sources and sinks. However, when implemented into a 3D GCM model taking into account the diffusive transport and exchange of methane between the regolith and the atmosphere, this process was found to induce only very small seasonal variations (a few % at most) [13]. This process, which can temporarily trap any sporadic excess of atmospheric methane, was also shown to be unable to maintain a sufficient contrast between a hypothetical plume (such as observed by [3]) and the surrounding concentration level. This was needed to relax the condition that the local CH$_4$ source measured by [3] had to have been reactivated very recently if the atmospheric lifetime of CH$_4$ is long [13].

Following the detection by the SAM-TLS instrument of a strong CH$_4$ seasonal cycle, a sensitivity analysis using a 1D-model has been made to reevaluate the possible effect of adsorption [14]. It was found that the SAM-TLS measurements could be explained by a large adsorption enthalpy ($\Delta H_{ads}$ ~31.5 kJ mol$^{-1}$) and a long near-surface effective atmospheric dissipation timescale (> 17 sols).

Here, we explore the consequence of this newly proposed adsorption enthalpy on the seasonal and diurnal cycles of methane using a 3D GCM, both at the location of the Curiosity rover and at a global scale.

Modeling: We use the subsurface transport model described in [13], which is coupled to the LMDZ atmospheric GCM. It models the diffusion of methane in the porous regolith down to -26 m; it takes into account the temperature-dependent adsorption process (assuming an Arrhenius law, as shown by [12] and as generally valid for trace gases) and the kinetics of the adsorption process. Although the latter is experimentally unconstrained for the time being, its timescale can be varied to investigate its effect on the diurnal cycle. By default, it is set to a very short timescale, but it was also increased to 1 day. The soil specific surface area (SSA) is a free parameter, set to 17 m$^2$.g$^{-1}$ by default [15], but a larger value of 100 m$^2$.g$^{-1}$ was also explored. The model can incorporate production or destruction terms in the subsurface, or a flux at the base of the subsurface model. It can also simulate a direct injection of CH$_4$ into the atmosphere, e.g. to simulate a venting event. The morphology of Gale crater is not resolved in these simulations.

Results: As a first scenario, we did not prescribe any specific source of CH$_4$, and let the atmospheric methane (initially uniformly distributed) equilibrate with the regolith. The global abundance is scaled so that the annual average obtained in the region of Gale match the average level measured by SAM-TLS. We compare the results obtained with $|\Delta H_{ads}|$ ~18 and 31.5 kJ mol$^{-1}$. We find typical equilibration times of ~1.5 and ~5 martian years, respectively (although deeper layers have not reach equilibrium yet, they do not affect the seasonal cycle strongly). The variations of the near-surface CH$_4$ volume mixing ratio obtained in the region of Gale are represented in Fig. 1. While the “low adsorption” case does not show any strong seasonal variations, as expected from [13], the “high adsorption” scenario shows variations that start mimicking the SAM-TLS measurements, and that look very similar to the 1D results of [14], albeit with a smaller amplitude and for partly different reasons. However, at a global scale and in particular at high latitudes, the seasonal variations are even more drastic (Fig. 2a), as a consequence of the strong seasonal dependence of the (reversible) CH$_4$ flux (Fig. 2b). Such large concentrations have not been observed by TGO. At Gale, this scenario also leads to diurnal variations that can reach ~20% near $Ls = 80^\circ$ for an SSA = 17 m$^2$.g$^{-1}$ and even ~55% for an SSA = 100 m$^2$.g$^{-1}$ (Fig. 1).
Fig. 1: Seasonal cycle of CH₄ (near-surface vmr, norm. to the average value) predicted at the location of Gale Crater, for |ΔH_ads| ~ 18 kJ/mol and SSA = 17 m² g⁻¹ (“low adsorption”) and 31.5 kJ/mol – 100 m² g⁻¹ (“high adsorption”). The SAM-TLS data (enriched mode) are shown for comparison.

As a second scenario, we simulated the injection of a short (24h) pulse of CH₄ at the location of Gale crater (directly into the lowest atmospheric cell) in an initially CH₄-free atmosphere and regolith, assuming an unlimited atmospheric lifetime. It confirmed that even if methane is strongly adsorbed and would ultimately be almost fully trapped in the regolith, the atmospheric dispersion of methane is much more rapid than its uptake by the regolith (methane is almost uniformly mixed after ~2 months). Even in the “high adsorption” scenario, the regolith is therefore inefficient at scavenging CH₄ and reducing its dispersion from the emission point. Ultimately, this scenario converges towards the first scenario, with smaller seasonal variations obtained at Gale than at high latitudes.

As a third scenario, we simulated a continuous source of CH₄ at the location of Gale crater, in an initially CH₄-free atmosphere and regolith, with a short atmospheric lifetime of 1 day. Even with such a short lifetime, the atmospheric dispersion of CH₄ is quite significant. As anticipated from the previous scenarios, a strong adsorption does not affect this result, as the timescale for adsorption is much longer than the atmospheric dispersion. Given the current coverage of TGO observations [9], a very short lifetime, of the order of 1-sol, is therefore necessary to reconcile the current TGO and MSL observations (Fig. 3). However, with such a scenario, the diurnal variations obtained at Gale become much more pronounced than the seasonal ones, making the SAM-TLS measurements much more sensitive to the time-of-day of sampling than to the time-of-year.

Conclusion: Leaving aside the difficulty to reconcile the TGO and SAM-TLS + Mars Express PFS observations with our current knowledge of the chemistry of the martian atmosphere, it appears that a strong adsorption process is a good candidate to explain the seasonal variations observed by SAM-TLS, although the adsorption enthalpy necessary for this process to be efficient is beyond the range of what has been measured so far in the laboratory (15-25 kJ mol⁻¹, see [12]). Depending on the scenario chosen for the location of the source (local or undefined), this process can induce quite distinct diurnal variations. Even in case of no specific CH₄ source location (scenario 1), the amplitude of such variations can reach 20-55% at specific times of the year at Gale, if the adsorption timescale is fast. Monitoring the diurnal cycle of CH₄ in addition to the seasonal one would therefore be useful to further constrain the location of methane emissions and the physical properties of the regolith affecting the adsorption process, including the adsorption/desorption timescale.


**Introduction:** The importance of regolith-atmosphere exchange in the diurnal, seasonal and inter-annual variability of the martian water cycle remains an open question, although there is a consensus on its fundamental role over geological timescales. Migration of ice across the planet upon variations of Mars’ orbital parameters and obliquity is one of the most significant geological processes that are still active and continuously reshaping the surface of the planet.

Theoretical/numerical studies have studied the subsurface ice stability over geological timescales [1-5] and over the seasonal cycle [4,6]; theories or simplified static models have tried to explain the current distribution of water-equivalent hydrogen measured by Mars Odyssey (confirmed in situ by the Phoenix lander) in terms of topographic control [7], transient ground ice [8], or exchange with hydrous minerals [9]; 1D or simplified 3D models of the ‘breathing’ of the regolith caused by adsorption of water vapor on the soil matrix have been developed to explain the diurnal variations of the water column density measured from the orbit [10] and of the H$_2$O volume mixing ratio measured at the surface of Gale crater by the REMS suite [11].

A growing number of studies has also been filling the need for experimental data on the adsorption or hydration properties of martian regolith simulants [12-18], on the diffusion of water vapor through such porous media [19, 20] and on the thermal properties of ice-rich materials under martian conditions [21]. These studies have enabled us to gain much insight into the dynamics of sublimation of a subsurface ice table and on the possible exchange of water vapor with the regolith.

Direct analyses of the martian soil by Curiosity have also provided new mineralogical and chemical constraints about the possible phase(s) that can be involved in the exchange of water vapor [22-24].

**Open questions:** Despite all these studies, many questions on this topic remain unanswered: how did subsurface ice at high latitudes exist? How did this ice evolve and migrate over time between polar, equatorial and mid-latitude regions? What is the nature of the hydrogen measured at mid- and low-latitudes by Mars Odyssey? Does it reflect long-term alteration of minerals by adsorbed water or frost? How can we reconcile the fact that simulations of the atmospheric water cycle without an “active” regolith fit the atmospheric observations pretty well, while the regolith contains a significant proportion of hydrated amorphous component, whose terrestrial analogs are known to be very hygroscopic and likely to exchange large amounts of water vapor [ref.?] More generally, how important is the role played by the regolith in the current and past water cycles?

**Previous studies done with GCM models:** To get a full and integrated view of all the processes that are involved, it is necessary to use a Global Circulation Model that describes the exchange of water with the perennial and seasonal polar caps, and its inter-hemispheric transport. Other GCMs interacting with an active regolith have been developed in the past [25, 26], but their model of regolith was quite simple (2-layers model and no formation of subsurface ice in [26]) and gave conflicting results on its importance on the current water cycle. Böttger et al. [6] have implemented a more complex regolith scheme in the LMD Global Climate Model [27] and their results, although dependent upon initial conditions, demonstrated the potential importance of regolith-atmosphere exchange on the seasonal and inter-annual water cycle. For instance, they found that the regolith can act as a buffer for water vapor leaving the northern high mid-latitudes during northern summer, preventing some of the water from reaching the southern hemisphere via the Hadley circulation and thus enabling to maintain the observed North-South atmospheric water vapor asymmetry. This water, trapped in the soil during winter, is then released into the northern spring time atmosphere and returns to the residual water ice cap through eddy transport. An active regolith had therefore a stabilizing effect on the simulated water cycle. However, they were unable to explain the purported diurnal variations of the water column abundance by exchange with the regolith. The same subsurface model has been used to evaluate the evolution of the subsurface ice reservoirs over recent geological times [5].

Here, we upgraded the subsurface model developed by [28], which is coupled to the LMDZ GCM [27]. The latter incorporates improved cloud microphysics [29], and its description of the water cycle has been revised by parametrizing sub-grid scale clouds [30] and by refining its vertical resolution [31].

**Description of the subsurface model:** The model, which is coupled to the subsurface thermal model, simulates the diffusion, adsorption and condensation of water molecules within the soil. It is an implicit model. It is purely diffusive (it does not take into account advection, surface diffusion, barodiffusion and thermal transpiration). The model uses either the H$_2$O atmospheric mixing ratio as boundary condition, or the ice saturation...
pressure if water ice is present on the surface. The diffusion coefficient (in a transition regime between Knudsen and molecular diffusion) takes into account the obstruction of the pores by ice, following the numerical work by [32]. The equilibrium between the vapor and adsorbed phases is described by a Langmuir-type of isotherm, but linearized versions of Type II and III isotherms, which are simplified versions of the isotherms measured by [12] are being implemented. Unlike existing models, the kinetics of the adsorption process can also be taken into account. Although it has not yet been well constrained experimentally, its influence on the diurnal cycle can be investigated. The soil specific surface area (SSA) and the adsorption enthalpy are free parameters of the model. A feedback of the ice content on the thermal properties of the regolith can also be activated, based on the experimental results of [21].

Results: Since the regolith can potentially hold a very large amount of water, a critical step needed before coupling the subsurface model to the atmospheric cycle is the initialization of the subsurface water reservoir. Since the current atmospheric model matches the observations pretty well, we decided for this initialization to force the regolith to equilibrate with the H2O cycle obtained without an active regolith, by imposing time-variable near-surface H2O mixing ratios as boundary condition to the subsurface model. Small deviations from this initial state can then be explored. This procedure allows us to make predictions of the distribution of stable subsurface ice, both in terms of geographical extent and depth to the ice table (Fig. 1, 2). It can also be used to extract the time evolution of the ice content as a function of depth, to estimate timescales of ice growth and to extrapolate the ice filling process to geological times. It can also be used to make predictions of global H2O maps for different adsorption isotherms (Fig. 3), to be compared to the actual H2O map derived by Mars Odyssey GRS.

From these initial states, we will explore the sensitivity of the H2O atmospheric cycle (diurnal and seasonal) to different types of adsorption properties. Conversely, a comparison to the observed atmospheric water cycle should provide constraints on these properties. We will also explore the sensitivity of the diurnal and seasonal cycles on the kinetics of the adsorption/desorption process.