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## Post-print: Retrieval of Mars CH<sub>4</sub> Gas Spatial Density Distribution

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**Date:** 2017-03-10T00:00:00+00:00

### Abstract

Currently, the detection of CH<sub>4</sub> gas on Mars constitutes a crucial approach in the search for life on Mars. Delineating the locations of CH<sub>4</sub> source regions on the Martian surface can enable the selection of appropriate target sites for future life exploration endeavors. Based on the detection of resonant scattering of Martian CH<sub>4</sub> gas, this study retrieves the spatial distribution of CH<sub>4</sub> gas on Mars through numerical simulation. The inversion results can reproduce the model's density distribution, identify regions with relatively dense CH<sub>4</sub> gas density distributions, and thus enable the determination of the locations of CH<sub>4</sub> source regions on the Martian surface.

### Full Text

### Preamble

#### Inversion of the Spatial Density Distribution of Martian CH<sub>4</sub> Gas

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Funded by the National Natural Science Foundation of China (41231066, 41174145) and the Special Fund of the State Key Laboratory of Space Weather.

## Abstract

Current detection of Martian CH<sub>4</sub> gas serves as an important means of exploring potential life on Mars. Identifying the locations of CH<sub>4</sub> source regions on the Martian surface can help select appropriate target sites for future astrobiological exploration. This paper investigates the spatial distribution of Martian CH<sub>4</sub> gas through numerical simulation based on detecting its resonant scattering. The inversion results can reproduce the modeled density distribution, identify regions with relatively dense CH<sub>4</sub> concentrations, and thereby determine the locations of CH<sub>4</sub> source regions on the Martian surface.

**Keywords:** Mars, CH<sub>4</sub>, Inversion, CT

## Introduction

The search for extraterrestrial life has been a persistent scientific endeavor. In 2008, NASA's Phoenix Mars Lander discovered water ice on the Martian surface, establishing the necessary conditions for life [1]. In future Mars exploration missions, discovering whether life currently exists or existed in the past would represent a groundbreaking achievement.

On Earth, 90% of CH<sub>4</sub> gas is released through biological digestion processes. While CH<sub>4</sub> has been confirmed in the Martian atmosphere, its biological origin remains unverified [2]. Consequently, detecting Martian CH<sub>4</sub> has become a crucial method for exploring potential life on Mars.

Current observations indicate that CH<sub>4</sub> concentrations in the Martian atmosphere are approximately one part per billion [3], though this represents only a global average. If we could determine the global spatial density distribution of CH<sub>4</sub>, we could locate the regions with the highest concentrations and thereby delineate CH<sub>4</sub> source regions on the Martian surface. This would provide essential scientific guidance for selecting optimal target sites in future astrobiological exploration.

In deep space exploration, detecting characteristic spectral lines produced by gas molecules through resonant scattering has a long history [4]. Drossart et al. identified CH<sub>4</sub> molecular fluorescence spectra in studies of Jupiter and Saturn. In 1995, the European Space Agency's Infrared Space Observatory became the first satellite to successfully detect CH<sub>4</sub> fluorescence in the infrared band [5]. Our research group is currently investigating methods to detect resonant scattering from Martian CH<sub>4</sub> gas, and this work builds upon that foundation.

Due to the tenuous nature of Martian CH<sub>4</sub> and the absence of secondary scattering, the atmosphere can be approximated as optically thin. Data obtained by the detector represents a line integral of CH<sub>4</sub> resonant scattering intensity along the observation path, which is proportional to the CH<sub>4</sub> column density in that direction. This relationship can be expressed as:

$$I(\lambda) = \int_0^L n(\lambda) \sigma(\lambda) ds$$

where  $(\ )$  represents the data detected by the detector along direction  $(\ )$  is the CH density at spatial location  $(\ )$ , and  $(\ )$  is a proportionality factor.

This process is consistent with the projection process in Emission Computed Tomography (ECT). When a satellite observes Martian CH from different angles, CT (Computed Tomography) methods can be employed to invert the spatial distribution of CH. This paper uses numerical simulation to invert the spatial density distribution of CH using CT methods and compares the results with a predefined CH density model, thereby providing theoretical support for observational planning.

## 1 CH Model

Due to limited observational data, current Martian atmospheric models do not include CH. Therefore, we must establish a predefined CH distribution model. Our model is constructed based on known patterns of Martian atmospheric distribution and may not perfectly match the actual CH spatial distribution. However, in CT reconstruction research, simulation models are commonly used to study inversion accuracy. These simulation models typically employ materials with densities similar to the research target and are designed according to the target's structure, meaning that algorithm effectiveness does not fundamentally change with model variations. In other words, if future satellite data volumes match those used in our simulations, the inversion accuracy will be comparable to that achieved with our model.

We utilize atmospheric distribution data from the Mars Climate Database (MCD). MCD 4.3 includes meteorological data from the Martian surface to over 250 km altitude, encompassing temperature, wind fields, pressure, radiation flux, and atmospheric composition (dust, water vapor, ice content). This database derives from Mars atmospheric GCM (General Circulation Model) results that closely match observational data, providing accurate vertical profiles of CO, N, O, and CO volume ratios at different locations. Using MCD, we first calculate the total atmospheric mass density and the vertical distribution of volume ratios for CO, N, O, CO, O, ice, and water vapor at each longitude and latitude, where volume ratio equals the number density of a component divided by the total atmospheric number density.

Based on this atmospheric data, we make the following assumptions: First, CH is not globally uniformly distributed but maintains a constant volume ratio of 10 ppb with altitude. The CH volume ratio follows a Maxwellian distribution with longitude and latitude. Second, since CH constitutes an extremely small fraction of the atmosphere, we ignore its contribution to the total atmospheric mass density. Under these assumptions, we calculate the total atmospheric number density from the total mass density and then determine CH number density at different longitudes, latitudes, and altitudes according to the CH volume ratio.

Based on existing observations, we assume CH distribution is primarily con-

centrated in low-latitude regions. Therefore, our model restricts the CH distribution to specific latitude and longitude ranges. Since the satellite orbit is a polar orbit in the dawn-dusk plane (see Section 3.1), Mars' rotation ensures uniform inversion accuracy across all longitudes. To reduce computational load, the model includes only E to 2 E longitude, centered at (6 E). Additionally, CH density decreases with decreasing pressure, and the inversion aims to capture this diffusion process to ultimately identify source regions—areas with the densest concentrations. To minimize computation, the model limits CH distribution altitudes from the Martian surface to 150 km. As shown in [Figure 1: see original paper] (displaying the natural logarithm of density), the maximum density occurs near the model center at the surface (6E), with a value of  $9 \times 10^{-3}$ .

## 2 Inversion Method

Strictly speaking, accurate inversion requires projection lines passing through the object to cover a  $180^\circ$  angular range (known as the projection data completeness condition) [6,7]. However, this condition is rarely satisfied in practice, preventing exact inversion results. Nevertheless, compensation methods incorporating prior knowledge can improve inversion accuracy.

CT theory has matured over decades and been successfully applied across various fields. For complete projection data, exact inversion algorithms such as PI-lines [8] and Filtered Back-Projection (FBP) [9] can be used. When projection data is incomplete, iterative algorithms like Algebraic Reconstruction Techniques (ART) [10,11] and Gradient Projection (GP) [12,13] are typically employed. In 2006, Sidky et al. [14] combined Total Variation (TV) minimization with the widely-used ART algorithm, achieving excellent results for CT inversion with severely limited projection data. Since satellites observing Martian CH gas cannot easily acquire complete projection data, this paper adopts this combined method for numerical simulation.

### 2.1 ART Algorithm

The essence of the ART algorithm is solving a system of linear equations. When a detector at spatial position observes the reconstruction target, each detector's measurement and the region to be inverted can be expressed as:

where  $\mathbf{d}$  is the vector of voxel density values in the reconstruction region,  $\mathbf{m}$  is the measurement from detector  $i$ , and  $\mathbf{p}_i$  is the corresponding projection matrix vector. Combining measurements from all positions yields:

ART begins by assuming an initial value  $\mathbf{x}^{(0)}$ , then calculates the first approximation  $\mathbf{x}^{(1)}$ , followed by a second approximation  $\mathbf{x}^{(2)}$  from (1), and continues iteratively until convergence criteria are met. When calculating  $\mathbf{x}^{(k)}$  from  $\mathbf{x}^{(k-1)}$ , the following correction formula is used:

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + \frac{\mathbf{m}_i - \mathbf{p}_i^T \mathbf{x}^{(k-1)}}{\mathbf{p}_i^T \mathbf{p}_i} \mathbf{p}_i$$

where  $\alpha$  is the relaxation factor.

## 2.2 TV Method

Total Variation was first proposed by Rudin et al. for image denoising and has since become a widely used optimization criterion for improving CT image reconstruction quality.

Introducing TV constraints into the ART algorithm involves solving an optimization problem that minimizes image total variation under projection equation constraints:

$$\|f - \hat{f}\| + \lambda \sum_{i,j,k} \sqrt{|f_{i,j,k} - \hat{f}_{i,j,k}|^2 + \epsilon^2}$$

By incorporating prior conditions into the ART algorithm (for Martian CH<sub>4</sub> inversion, these conditions are: non-negative density values; if a value on a projection ray is zero, then all voxels intersected by that ray have zero density), TV constraints yield improved reconstruction images when projection data is incomplete.

## 3 Selection of Calculation Parameters

Our research group has adopted the following design parameters for the satellite orbit and detector.

### 3.1 Satellite Orbit Parameters

In the simulation, CH<sub>4</sub> gas is assumed to rotate with Mars, with no change in its density distribution over several days. Therefore, a Mars-synchronous satellite cannot observe CH<sub>4</sub> from all surface regions. A polar orbit enables observation of all regions as Mars rotates. For computational simplicity, a circular orbit is adopted. To describe the satellite's orbit conveniently, we define a Mars-Solar coordinate system (MS): the origin is at Mars' center, the X<sub>MS</sub> axis points toward the Sun, the Y<sub>MS</sub> axis points toward Mars' dusk side, and the Z<sub>MS</sub> axis follows the right-hand rule. To prevent direct sunlight from striking the detector, the satellite orbit is placed in the dawn-dusk Y<sub>MS</sub>-Z<sub>MS</sub> plane.

In the model, the maximum altitude of CH<sub>4</sub> gas distribution is 69 km. To ensure that each detector unit can observe all CH<sub>4</sub> along its line of sight from any orbital position, the satellite altitude is set to 100 km, with an orbital period of 24.6 hours.

### 3.2 Detector Parameters

In the simulation, the detector's field-of-view is set to 180° to ensure observation of all CH<sub>4</sub> gas from any orbital position, except for regions occluded by Mars (occlusion occurs in two forms: direct occlusion, where the line-of-sight integral of resonant scattering intensity terminates at the near side of Mars, preventing detection of CH<sub>4</sub> on the far side; and indirect occlusion, where CH<sub>4</sub> on the far side does not interact with sunlight, making it undetectable). Each detector

unit has a field-of-view of  $^{\circ}$  (corresponding to horizontal and vertical resolutions of 50 km, which represents the current capability of our detector development), resulting in  $45\times$  detector units. During observation, the detector center points toward Mars' center, with a sampling interval of 1.5 minutes and total data acquisition time of one Martian rotation period (approximately 2 h), as the satellite' s trajectory repeats every 2 h in Mars-fixed coordinates, as shown in [Figure 2: see original paper].

#### 4 Numerical Simulation Results

The inversion spatial range completely covers the CH distribution region in the model, extending from the Martian surface at 79 72 k to 9 72 k altitude. In the inversion, longitude and latitude grids are spaced every  $^{\circ}$ , with altitude layers every k (18 layers total), yielding  $8 \times 8 \times 6$  grid cells. The inversion results are shown in [Figure 3: see original paper]. The reconstructed CH is primarily concentrated between latitudes and longitudes E to 2 E , closely matching the original model.

For further comparison, we analyze two cross-sections at  $0^{\circ}$  latitude and  $60^{\circ}$  longitude, shown in the upper and lower panels of [Figure 4: see original paper], respectively. The left column shows the model, and the right column shows the inversion results. These figures clearly demonstrate that CH is confined within latitude and longitude E to 2 E , with density decreasing with altitude at constant latitude and longitude, consistent with the model. However, the inverted densities are overestimated, particularly at higher altitudes, primarily due to insufficient projection data. As shown in [Figure 2: see original paper], the satellite trajectory has large longitudinal gaps, reaching up to  $2^{\circ}$  in the equatorial plane, resulting in significant data deficiencies. Additionally, Mars' occlusion contributes to projection data loss.

If the camera sampling interval could be reduced, more projection data would be available, improving inversion accuracy. Halving the sampling interval from 1.5 minutes to 0.75 minutes reduces the average error (defined as the ratio of the mean difference between inverted and original data to the mean original data) from 16.95% to 15.07%. Furthermore, considering satellite precession can also improve accuracy. In our calculations, we assume a simple precession of  $3^{\circ}$  per day. Due to this precession, the satellite' s trajectory does not repeat in Mars-fixed coordinates. Given CH ' s continuous spatial diffusion, observation duration should not be excessive; we therefore collected only 3 days of data, with orbital inclination varying gradually from  $85^{\circ}$  to  $9^{\circ}$ . With sampling intervals of 1.5 minutes and 0.75 minutes, the average inversion errors are 15.89% and 14.34%, respectively. compares these four inversion scenarios, demonstrating that increased data volume, smaller sampling intervals, or orbital precession all improve inversion accuracy.

## 5 Conclusions and Discussion

This paper presents numerical simulations of Martian CH<sub>4</sub> spatial distribution inversion using CT methods. The results show that when a satellite operates in a circular dawn-dusk orbit, the inverted density distribution agrees well with the model, particularly in terms of density variation trends. The inversion clearly identifies regions with relatively dense CH<sub>4</sub> concentrations, fulfilling the scientific objective of “delineating CH<sub>4</sub> source regions to select appropriate targets for future astrobiological exploration.”

However, several issues remain. First, the inversion exhibits some deviation. Only increased sampling data volume (through reduced sampling intervals or orbital variations) can improve accuracy. Second, the spatial resolution of inversion results needs improvement, as it is constrained by detector resolution. Our simulations are based on the current detector design capability (50 km horizontal and vertical resolution), which is limited. Enhancing detector resolution is an ongoing challenge for our group. Third, this study considers only steady-state conditions, whereas in reality, Martian neutral winds affect CH<sub>4</sub> distribution, causing temporal variations. Our group will address these issues in future work to achieve optimal reconstruction performance.

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