Data processing of the active neutron experiment DAN for a Martian regolith investigation


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1. Introduction

At 10:32 p.m. PDT on August 5, 2012 the NASA Mars Science Laboratory (MSL) rover named Curiosity successfully landed in Gale Crater in the equatorial region of Mars. One of the main tasks of the Curiosity rover mission is the investigation of the historical and current amount of water present in the regolith at Gale Crater. Several rover instruments on board Curiosity are able to detect H, OH and H₂O in regolith samples [1]. Most of these instruments perform remote analysis of a small spot on the surface or take a regolith samples for laboratory analysis inside the rover. All samples are delivered for the analysis to Chemistry and Mineralogy (ChemMin) X-ray diffraction (XRD) and X-ray fluorescence (XRF) instrument [2] and to the Sample Analysis at Mars (SAM) quadrupole mass spectrometer/gas chromatograph/tunable laser spectrometer suite of instruments [3]. These observations are also supported by the Alpha Particle X-ray Spectrometer (APXS) provided remote X-ray spectroscopic analysis of a sample to determine the relative abundances of different rockforming elements [4], by the Chemistry and Camera (ChemCam) instrument developed to vaporize thin layers of material from Martian soils by a laser beam to identify the elemental composition and an optical camera to capture detailed images of the area analyzed [5] and by multiband observation with the Mast Camera (Mastcam), which are sensitive to the presence of some hydrated minerals [6]. Dynamic Albedo of Neutrons (DAN) [7–11] is the only instrument on board the rover that provides information about the subsurface water concentration and its vertical distribution within a large volume of regolith just below the rover.

The DAN instrument has been developed by the Space Research Institute (IKI) and has been contributed to the NASA MSL mission by the Russian Space Agency. The instrument has a direct heritage from High Energy Neutron Detector (HEND) instrument, which was also developed by IKI, as part of the Gamma Ray Spectrometer...
(GRS) suite on board NASA’s Mars Odyssey [12,13] orbiter. The HEND instrument, still operating on the orbit, measures fluxes of thermal, epithermal and fast neutrons produced in the Martian subsurface by energetic particles of Galactic Cosmic Rays (GCRs). Using these data, it is possible to determine the water content in the regolith down to about 1 m in depth below the surface. A global map of ground water distribution on Mars is the main result obtained using the HEND data [13,14]. Due to the relatively high orbit of Mars Odyssey (at about 450 km altitude), the HEND’s field of view (FOV) is about 300 km in radius, which is too broad for water mapping inside individual craters, even as large as the 154 km Gale Crater. A similar limitation of spatial resolution will occur for any orbital neutron measuring instrument because, due to mass limitations, it is not possible to design an orbital neutron detector with spatial resolution better than several tens of kilometers with reasonable instrument mass and signal integration time. Nevertheless, it is useful to know the hydrogen/water distribution in the region where a lander or rover may operate on the Martian surface so as to better understand the local regolith properties and to ultimately select the best sites for detailed studies. The DAN instrument has been selected for the Curiosity payload to characterize the presence of ground water in the local subsurface regolith along the rover traverse.

The concept of the DAN experiment is based on a well-known method of nuclear physics for remote determination of hydrogen abundance—active neutron logging (see, for example, [15]). This method is based on a pulsing irradiation of a regolith sample with high energy neutrons. Traveling in the sample, these neutrons interact with nuclei in elastic and inelastic processes and lose energy (slow down or moderate) with some being absorbed by the nuclei, producing gamma-ray emission (sometimes together with α, p, β, γ, secondary n). Such interactions of neutrons occur with the nuclei of all elements of the regolith. The moderation of scattered neutrons is most efficient when the masses of the neutron and the nucleus are close. The energy transfer becomes less efficient in cases where a neutron collides with a massive nucleus. Due to the fact that the mass of a neutron is practically equal (difference is about 0.14%) to the mass of a hydrogen nucleus (a proton), the presence of even a small amount of hydrogen in the regolith makes neutron moderation in the subsurface much more efficient in comparison to a regolith without hydrogen.

After each pulse of high energy neutron irradiation made by the PNG, a large number of thermal, epithermal and fast neutrons have a chance to escape from the regolith subsurface and be detected. In the case of a regolith with a significant amount of hydrogen, injected neutrons are slowed down more quickly and a large part of the detected neutrons are moderated down to thermal energies. Conversely, in the case of a regolith with a negligibly small amount of hydrogen, the main fraction of detected neutrons will have epithermal energy. Therefore, separate measurements of thermal and epithermal neutrons allow one to determine the hydrogen concentration in the regolith.

Generally, water distribution in the subsurface regolith is not uniform for a number of reasons. One reason is the exposure of the regolith to a dry atmosphere of Mars. Such contact leads to very rapid evaporation of water from the top regolith layer, making it drier than the deeper soil layer. In this case, the high energy neutrons injected into the subsurface regolith by the instrument must go some distance before they reach a depth where a hydrogen-rich layer of regolith is located. Traveling into this layer of regolith, and interacting with nuclei, the neutrons are effectively slowed down to thermal and epithermal energies. Some moderated neutrons may return to the regolith surface, leave it, and be registered by the instrument detectors. Taking into account the small speed of these neutrons and the distance that they have to go to be detected, it is obvious that they will be registered some later than the rare neutrons that were moderated in the top, dry regolith layer. Using short pulses of high energy neutrons and measuring the shape of thermal and epithermal neutron echo time history, one may determine the thickness of the top, dry regolith layer and the water amount in both the top and bottom layers. During diffusion into the regolith, some neutrons may also be absorbed by nuclei with large absorption cross-sections. In the Martian regolith, chlorine and iron are known to be the main nuclei with large neutron interaction cross-sections [16,11]. This absorption effect is stronger for slower neutrons, and it also can be observed by the neutron instrument with separate detectors of thermal and epithermal neutrons.

As is common for nuclear science, DAN active measurements of the Martian regolith do not directly provide the physical parameters of the regolith composition. One needs to perform a comprehensive program of data analysis with DAN observations to extract data about the content of water and neutron-absorbing elements in the soil. The main goal of this paper is to describe the methods of data processing for determining the water concentration and its depth distribution. The short DAN experiment description is presented in Section 2, methods used for processing the DAN data gathered during active measurements are described in Section 3, numerical simulations of DAN active measurements are presented in Section 4, Section 5 describes data analysis of the DAN active measurements for determining hydrogen distribution parameters, abundance of neutron-absorption elements and their uncertainties. DAN experiment data products available at the Planetary Data System (PDS) are described at Section 6. Conclusions are presented in Section 7.

2. Overview of DAN investigation

2.1. The DAN instrument description

The DAN PNG module (Pulsing Neutron Generator) emits an omnidirectional pulse of about 10⁷ neutrons per short, 2 μs, pulse. It uses a small charged particle accelerator to accelerate deuterium ions (2D⁺) toward a target impregnated with the hydrogen isotope tritium (3T) to generate neutrons in the reaction: 2D⁺ + 3T→ 4He+ + n + 176 MeV. The neutron from this reaction takes 14.1 MeV and the alpha-particle takes 3.5 MeV.

To measure the dynamic albedo of neutrons from the regolith, the DAN instrument includes the DAN DE (Detectors and Electronics) module which consists of analog and digital electronics, power supply units and two 3He proportional counters with a gas pressure of 3 atmospheres: one counter with Cd (detector CTN) and one with Pb (detector CTN enclosures). The CTN detector measures neutrons within a broad energy range from about zero up to ~1 keV, while the CETN detector measures epithermal neutrons in the energy range from ~0.4 eV (which is energy of cadmium transparency for slow neutrons) up to ~1 keV. The upper limit of both detectors’ sensitivity, about 1 keV, is defined as the energy at which neutron detection efficiency drops below 1% of maximum efficiency of the detector without any enclosure [9]. The difference of CTN and CETN neutron counting rates provides information about the neutron flux below the energy of 0.4 eV. One may consider this flux as mainly contributed by thermal neutrons (energy ~kT, where k is the Boltzmann constant and T is the temperature of the regolith).

DAN operates in passive and active modes according to commands from the Earth. In the passive mode the instrument measures the neutron albedo of the soil produced by neutrons generated by the Curiosity rover MMRTG (Multi Mission Radioisotope Thermoelectric Generator) and by energetic particles of Galactic Cosmic Rays (GCR) interacting with the Martian regolith.
It is possible to determine an in-depth average hydrogen concentration in the regolith using these data [17].

In the active mode, the DAN PNG emits pulses of fast neutrons and DAN DE proportional counters detect the time-dependent dynamic albedo of neutrons of the regolith. The hydrogen concentration, its depth distribution and other regolith properties may be found from such tests, however, the physics of DAN measurements do not allow one to distinguish in which form hydrogen exists in the regolith: free water ice, chemically bound water, hydroxide, methylene, etc. Neutron logging allows one to characterize the elemental abundance, but not the chemical composition of the regolith. Since it is commonly accepted that water is the main hydrogen bearing chemical substance in the Martian regolith, it is practical to convert the hydrogen concentration found from the DAN data analysis into water equivalent hydrogen (WEH) concentration in the regolith. Therefore, when the hydrogen content is considered, it refers to the water equivalent hydrogen.

2.2. Nuclear reactions of DAN subsurface sensing

Neutrons interact with the regolith in a number of nuclear reactions, which are characterized by corresponding cross-sections. Two groups of these interactions are the most important for the DAN data interpretation: neutron scattering and absorption. Each of these interactions may be also divided into two types. Neutron scattering may be elastic or inelastic. In the case of inelastic scattering, a portion of the initial neutron energy goes into exciting the target nucleus. During de-excitation, the target nucleus usually produces characteristic gamma rays. Inelastic scattering reactions have an energy threshold—if the initial neutron energy is less than the energy of the excited state, the reaction cannot take place.

In the case of elastic scattering, there is energy conservation for the incoming and outgoing particles, neutron and nucleus. However, due to momentum conservation, a fast neutron loses energy in its interaction with the at-rest nucleus of mass \( M \) (masses are measured in unified atomic mass units, the neutron mass is equal to 1.008664916 amu). After scattering at angle, \( \theta \), in the center of mass system, the neutron energy, \( E \), is related to the initial neutron energy \( E_0 \) by the expression:

\[
\frac{E}{E_0} = \frac{\Delta^2 + 2 \Delta \cos \theta + 1}{(\Delta + 1)^2}
\]

The energy \( E \) is minimal if the scattering angle \( \theta = 180^\circ \). Therefore, after elastic scattering, the neutron will have energy \( E \) in a range from \( E_0 / (\Delta - 1 / (\Delta + 1)^2) \) to \( E_0 \) depending on the scattering angle, \( \theta \). For most chemical elements with \( \Delta > 16 \), the maximal energy reduction in one neutron scattering event with a nucleus is less than 22%. But the neutron can lose up to its entire initial energy in a single interaction with hydrogen. This property of neutron scattering on hydrogen nuclei is exploited in neutron sensing experiments to determine the hydrogen abundance in materials.

The neutron absorption reactions may also be divided into two types: radiative capture and particle production. In the particle production reactions the initial neutron is absorbed by a nucleus with an emission of protons, secondary neutrons, \( \alpha \)-particles, etc. Usually, this type of reaction is possible only for high energy neutrons. In radiative capture reactions, the initial neutron is absorbed by a nucleus producing a new, excited, nucleus. The new nucleus de-excites instantly, emitting characteristic gamma rays. The radiative capture reaction is known also as thermal neutron absorption because its cross-section increases with decreasing neutron energy and achieves a maximal value at the lowest neutron energy. The cross-section of these reactions varies across a wide range from nucleus to nucleus. There are some isotopes with very large thermal neutron absorption cross-section: \(^{157}\text{Gd}, ^{155}\text{Gd}, ^{140}\text{Sm}, ^{115}\text{Cd}, ^{151}\text{Eu}, ^{9}\text{He}, ^{10}\text{B}, ^{196}\text{Hg}, ^{184}\text{Os}, ^{164}\text{Dy}, \text{etc.} \) (in descending order of the cross-section). However, most of these elements are very rare in the regolith, and do not contribute significantly to the absorption of leaking neutrons from the Martian soil. The absorption cross-sections are much smaller for the elements more commonly found in regolith, such as Si, Fe, Mg, Al, Ca, O, Cl, etc., but these elements play a major role in neutron transport and absorption.

Only two of these, Fe and Cl, should be taken into account for considering the neutron absorption process in the Martian soil, because they have rather large neutron absorption cross-section and their concentration in the soil is sufficiently high [16,11]. The presence of neutron absorbers in the regolith changes the time-history of neutron albedo from the soil because leaking neutrons with lower energy have a higher probability for absorption. In the data processing of DAN active measurements, a special parameter is introduced to take into account all absorbers of thermal neutrons [see Sections 4.3 and 4.4].

2.3. Neutron die-away curves, as the main data products from DAN measurements

Active DAN measurements are performed only when the rover is stopped. The standard duration of active measurements is 15 min and the DAN pulsing frequency is 10 Hz (both values may be changed by commanding from Earth). During this time the DAN PNG produces 9000 neutron pulses. Following each neutron pulse, the DAN DE starts to measure the time-dependent albedo of neutrons from the local environment. Immediately after the pulse the instrument opens 64 successive logarithmic time bins and measures in these bins the counting rates from the CTN and CETN detectors separately (see Fig. 1). Length of the bins is described by geometric progression: \( \Delta t(t_i) = 5.0 \mu s \times 1.125^i \), where \( i \) varies from 0 to 63. After a single neutron pulse, the count statistics gathered in any of the 64 time bins are poor. It is obvious that a small number of neutrons detected after a single neutron pulse bring information about only some nuclei randomly distributed within subsurface with which these neutrons had interacted. From \( 10^7 \) neutrons emitted with each pulse, a significant

![Fig. 1. This scheme illustrates the dependence of the neutron flux of die-away curve vs. time after pulses. The 64 logarithmic time bins opened by the instrument's logic electronics to accumulate neutron counts are shown.](image-url)
fraction of these neutrons penetrate into the subsurface under the rover and interact with soil nuclei and lose energy in a number of different processes. Some of the moderated neutrons leak back out of the surface and only a small fraction of the neutrons reach the sensitive volume of the detectors. Therefore, to get detailed information about the average properties of a full volume of soil below the rover and to get measurements with a good signal-to-noise ratio, it is necessary to accumulate data gathered during many pulse-measurement cycles made at the same rover position. So, for the comprehensive science analysis DAN/DE electronics sums up counts in each time bin for the selected number of neutron pulses. With a large number of neutron pulses it resulted into the smooth time history of post-pulse neutron albedo from the regolith (also known as die-away curve). The selected number of 9000 neutron pulses for the one standard active measurement was found as a good compromise between high signal-to-noise ratio, strict radiation safety operation rules (overlapping of DAN active measurements with other instruments and rover systems activities) and limited power resources available onboard Curiosity rover.

Studying the shapes of die-away curves, one may determine the amount of hydrogen in the regolith and its distribution with depth. In general, the spectrum of neutron albedo from the regolith and its variability with time depends on a number of parameters like the regolith elemental composition, density, temperature and variability of these parameters with depth below the surface. The released data products of DAN active measurements are the discrete time profiles of neutron albedo counts \(N_{\text{tn}}(t_i)\) at the CTN (noted henceforth with the subscript \(\text{tn}\)) and CETN (noted henceforth with the subscript \(\text{etn}\)) sensors in 64 time bins after a pulse. It is important to remember that count statistics instruments like DAN that rely on nuclear interactions are different for example from an imaging instruments, where a CCD accumulates signal a one short exposure and provides an image which is practically ready for scientific analysis. DAN active measurements require time and detailed analysis (described below) before the regolith properties at a given rover location can be determined.

3. Initial processing of DAN rough active data

3.1. Background of DAN active measurements

Besides the pulsing DAN PNG, there are two other permanent sources of neutrons in the vicinity of the rover: the secondary emission of the soil due to irradiation by MSL MMRTG and the secondary emission of the soil due to bombardment by energetic particles of Galactic Cosmic rays (GCRs). The GCR flux varies in time due to solar activity. These variations are generally slow and smooth with ~11-year period or fast during Solar Particle Events with time scales from minutes to days. The GCR particles are primarily protons with energies \(> 100\, \text{MeV}\). They generate neutrons in the Martian atmosphere and regolith by spallation reactions. Most of these secondary neutrons have initially high energy \((> 20\, \text{MeV})\) and are able to produce additional charged particles and next generation of neutrons by nuclear interactions with the regolith and rover material. Neutron flux generated by the rover’s MMRTG is permanent and almost omnidirectional with energies from thermal energies up to \(\sim 10\, \text{MeV}\), peaking at \(\sim 3.1\, \text{MeV}\). These neutrons do not produce a significant amount of additional neutrons in the regolith and rover structures. Both type of neutrons – those generated by GCR or by the MMRTG – after interactions with the regolith and rover, may be detected by DAN. It was found that the neutron flux generated by the MMRTG is strong enough to dominate the DAN passive measurements (see [17] for more details). Counts produced by MMRTG and GCR should be considered as background and removed from the measured time history of post-pulse neutron albedo.

The background counting rate, \(B_{\text{tn,etn}}\), can be estimated separately for thermal and epithermal neutron detection as

\[
B_{\text{tn,etn}} = \frac{\sum_{i=1}^{n} P_{\text{tn,etn}}(t_i) \cdot \Delta T(t_i)}{\sum_{i=1}^{n} \Delta T(t_i)},
\]

where \(P_{\text{tn,etn}}(t_i) = N_{\text{tn,etn}}(t_i)/\Delta T(t_i)\) is the profile of raw count rate measured by the thermal (\(m\)) and epithermal (\(etn\)) neutron detectors in time bin \(t_i\) with duration \(\Delta T(t_i)\) for a range of indices from \(\rho_1\) to \(\rho_2\) at the instrument time scale, which corresponds to the time interval \(10^{-4} - 10^{-3}\, \mu\text{s}\) after the neutron pulse (there is practically no post-pulse emission of neutrons at these intervals). By subtracting \(B_{\text{tn,etn}}\) from all time bins of the measured die-away curves, one gets the pure die-away curves of neutron albedo, \(C_{\text{tn}}(t_i)\) and \(C_{\text{etn}}(t_i)\), for thermal and epithermal neutrons, respectively: \(C_{\text{tn,etn}}(t_i) = P_{\text{tn,etn}}(t_i) - B_{\text{tn,etn}}\) (see Fig. 2). This procedure removes all counts from constant sources (GCRs and MMRTG) and leaves only counts produced by neutrons generated by the DAN PNG, scattered in the regolith and/or rover structures and returned to the detectors.

3.2. Data normalization procedure

There are several factors influencing the intensity of die-away curves measured by the CTN and CETN detectors in addition to the regolith properties, which are the subject of investigations and change from place to place.

The first group of three factors is associated with non-stable performance of the PNG. The first is the spontaneous statistical fluctuations of the total number of irradiated neutrons from pulse to pulse. Usually, one active measurement is 15 min long, which corresponds to 9000 pulses at 10 Hz. To prepare the data for further analysis and to minimize the influence of individual pulse fluctuations, all 9000 measured die-away curves for each of the two detectors are averaged in each of the 64 post-pulse time bins.

The second factor is the degradation of the tritium-rich target in the DAN PNG with time, either due to bombardment by deuterium ions, or due to the tritium’s natural radioactive decay in the target. Due to this effect, the average number of neutrons generated per pulse continuously decreases with time. The third factor, which can change the neutron production rate during the pulse, is oxidation of the deuterium ion source’s surface by residual gas inside the DAN

![Fig. 2. A die-away curve measured by the CTN detector shown before (\(P_{\text{tn}}(t_i)\), blue line) and after (\(C_{\text{tn}}(t_i)\), red line) background subtraction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)](Image)
PNG vacuum tube. This leads to a situation where pulse intensity may be reduced after a long DAN PNG inactive period and will recover only after several tens of pulses.

The second and third factors lead to a finite lifetime of the DAN PNG—it is finite even if the instrument does not generate neutrons. The DAN PNG, developed by the N. L. Dukhov Institute of Automation (Moscow, Russia), has a “warranty period” of about 3 years from the date of manufacture. Taking into account the DAN instrument delivery, MSL pre-flight testing and cruise to Mars periods, the DAN PNG warranty expired at the end of August 2013, after about one year of MSL operations on the Martian surface. This does not suggest that the instrument will stop generating neutrons after this point. It has already continued successfully operating one additional year after the end of its formal lifetime. Thus, the decrease of the neutron pulse intensity cannot be predicted precisely. Fig. 3 shows the measured decrease of DAN PNG neutron production with time.

The second group of factors for changes in the counting rate of CTN and CETN detectors is the increase of the detectors’ efficiency with a time after the HV is powered on. This effect is described in [17]. Therefore, to look for the difference of DAN active data for different sites of the surface, one must exclude the variations of the pulsing intensity of PNG as well as the efficiency variations of the sensors. It is necessary to perform a special normalization of the measured data to compensate for all changes of counting rate which are not induced by variations of the regolith properties.

The time interval from 10 to 50 μs after the neutron pulse is used for this normalization. Numerical simulations have shown (see below) that during this time interval the DAN DE counting rate does not practically depend on the Martian regolith properties, but, instead, is dominated by neutrons back-scattered inside the rover mechanical structures close to the detectors and/or the neutron generator. This structure obviously remains the same during the mission, so the data at these bins may be used, as the reference values for normalization. To perform the normalization, all count rates measured by the CTN and CETN detectors within this time interval at a given rover location are summed independently:

$$M_{\text{DAN,etn}} = \sum_{i = \tau_1}^{\tau_2} C_{\text{DAN,etn}}(t_i)$$  (3)

where $C_{\text{DAN,etn}}(t_i)$—the count rates at the CTN and CETN detectors at $t_i$ time bin with the subtracted background, $\tau_1$ to $\tau_2$—interval of time bin indexes which correspond to the time range 10–50 μs after the neutron pulse. The uncertainty of $M_{\text{DAN,etn}}$ is

$$\Delta M_{\text{DAN,etn}} = \sqrt{\sum_{i = \tau_1}^{\tau_2} (\Delta C_{\text{DAN,etn}}(t_i))^2},$$

where $\Delta C_{\text{DAN,etn}}(t_i) = \sqrt{N_{\text{DAN,etn}}(t_i) \cdot \Delta T(t_i)}$—uncertainty of counting rates at CTN and CETN detectors at $t_i$ time bin.

For each Curiosity stop where DAN active measurements were performed, the values of $M_{\text{DAN,etn}}$ need to be found independently. Then, the measured die-away curve should be normalized using the found values:

$$A_{\text{DAN,etn}}(t_i) = \frac{C_{\text{DAN,etn}}(t_i)}{M_{\text{DAN,etn}}}.  \quad (4)$$

The statistical uncertainty $\sigma_{\text{DAN,etn}}(t_i)$ of the $A_{\text{DAN,etn}}(t_i)$ is based on the statistics of raw counts measured at ith time bin:

$$\sigma_{\text{DAN,etn}}(t_i) = \sqrt{\left(\frac{\Delta C_{\text{DAN,etn}}(t_i)}{M_{\text{DAN,etn}}}ight)^2 + \left(\frac{M_{\text{DAN,etn}} \cdot \Delta C_{\text{DAN,etn}}(t_i)}{(M_{\text{DAN,etn}})^2}\right)^2}.  \quad (5)$$

All effects from DAN PNG intensity variations and DAN DE efficiency changes are thought to be removed from the die-away curves by this normalization. The normalized profiles of die-away emission should only manifest the variations of neutron flux intensity produced by the regolith composition and/or hydrogen concentration variations.

4. The concept of DAN active data analysis

4.1. Discussion

After normalization is done, it is possible to use the measured die-away curves to compare them with the numerical model predictions to estimate the best fitting model parameters of the Martian regolith at selected rover stops. To get the regolith parameters, one has to perform a procedure of neutron data deconvolution which uses Monte Carlo numerical simulations of the DAN active measurements that compare simulations with the actual measurements. Typical soil model contains information about general soil structure, some fixed parameters (known from other measurements) and measurable parameters (like water concentration). The regolith model should be changed if the numerical model differs significantly from the measurements. One can accept the parameters of the modeled regolith if the numerical model is in good statistical agreement with the measurements.

To perform this procedure a numerical model of the instrument, the rover and Martian surface must be created. The model of the instrument should be evaluated and tested with results from the instrument comprehensive laboratory physical calibrations with well-known neutron sources, regolith samples and hydrogen and other elemental concentrations. Only then can the measured time profiles of neutron albedo (die-away curves) in the lab setting be compared with the numerical model predictions.

4.2. Neutron interactions numerical simulation code

For numerical modeling of neutron interactions with the Martian regolith and neutron registration by the detectors, the code MCNPX is used. The Monte Carlo N-Particle eXtended or MCNPX code, was developed at the Los Alamos National Laboratory (LANL) [18]. This code uses nuclear data tables and physics models to transport neutrons, protons, photons, electrons and about 30 additional particles (deuterons, tritons, alphas, pions, muons, etc.). Models of particle interactions with matter are used when no tabular data libraries are available or when the data are...
beyond the energy range of the data tables (higher than 20–150 MeV for neutrons). This code is able to perform three-dimensional and time dependent modeling of nuclear physics processes. MCNPX has proven itself (see, for example, [19]) and shown good results in modeling nuclear instruments for space missions at Mercury, the Moon, Mars and other celestial bodies (e.g. [20–22,13]).

4.3. Modeling of DAN neutrons emission and detection

To be able to compare neutron measurements on the Martian surface with numerical modeling of the DAN experiment, it is necessary to create a numerical description of the DAN DE and PNG modules, the MSL rover mechanical structures and the Martian regolith in the format of MCNPX input files. Modeling of the MSL structures and composition of the Martian regolith will be described in the next section of this paper.

The DAN PNG module is described as a point source of monoenergetic 14.1 MeV neutrons emitted isotropically. This source produces \( \sim 10^7 \) neutrons in one pulse. The shape of the pulse is shown on Fig. 4. Special numerical simulations were done to check whether the DAN PNG internal structure and housing produced a significant anisotropy or energy broadening of the 14.1 MeV neutron flux emitted by the PNG during a pulse. No significant effects were found and the above-mentioned simple description of the neutron sources for numerical simulations is therefore acceptable.

The DAN DE model for MCNPX was created using the instrument engineering drawings (Fig. 5). This model includes two \(^3\)He proportional neutron detectors with 3-atmosphere gas pressure: the counter of thermal neutrons (CTN) and the counter of epithermal neutrons (CETN). The CETN detector is surrounded by a cadmium (Cd) shield with a thickness of 1.0 mm; the CTN detector is surrounded by lead (Pb) shield with a thickness of 1.0 mm. The CETN is not sensitive to thermal neutrons with energies \(< 0.4 \text{ eV}\) due to a large capture cross-section of cadmium nuclei for such neutrons. The efficiency of the detectors is shown on Fig. 6 of [9]. The lead enclosure of the CTN detector shields it from being overloaded by bremsstrahlung X-rays emitted from the DAN PNG during a neutron pulse. There is a hole in each shielding enclosure for the high voltage power supply cable which is also taken into account in the model. A small amount of thermal neutrons may propagate through these holes and produce additional counts of thermal neutrons in the CETN detector. The electronic unit includes CTN and CETN detectors and electronic boards covered by high voltage insulating compound inside an aluminum alloy housing. The main electronic block contains both digital electronics, and low and high voltage power supply units for the detectors within an insulating compound. The electronic unit and main electronic block are both included in the model.

4.4. Numerical modeling of the Martian environment around DAN

The Martian environment around DAN is producing the neutron albedo from pulses of high energy neutrons by the DAN PNG. This environment consists of the Martian atmosphere and the Martian subsurface.

The Martian atmosphere has been modeled for all DAN active measurements at the bottom of the Gale, as a uniform carbon dioxide gas layer with a density of \(1.6 \times 10^{-5} \text{ g/cm}^3\) and temperature of 213 K (see Table 1). Results of modeling have shown that the total contribution of neutron albedo of the atmosphere is negligibly small in comparison with the surface (\(< 0.1\%)\). The diurnal and seasonal atmospheric variations produce even smaller effects on DAN active measurements of neutron albedo. Therefore, at the current stage, these variations are not taken into account.

The die-away curves of the neutron albedo of the regolith depend on the following physical properties: the density \( \rho \), the mass fractions, \( \xi_A \), of the soil-constituting chemical elements \( A \), the efficiency of neutron moderation, and the efficiency of neutron absorption.

![Fig. 4. Typical shape of a DAN PNG neutron pulse.](image)

![Fig. 5. Schematic cross-section of the DAN DE used for the numerical simulations.](image)

<table>
<thead>
<tr>
<th>Chemical element</th>
<th>Atmosphere</th>
<th>Regolith</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>26.44 wt%</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>2.81 wt%</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>70.59 wt%</td>
<td>44.30 wt%</td>
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<td>Na</td>
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<tr>
<td>Al</td>
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<td>Si</td>
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</tr>
<tr>
<td>P</td>
<td>0.54 wt%</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>3.79 wt%</td>
<td></td>
</tr>
<tr>
<td>Cl</td>
<td>Variable</td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td>0.16 wt%</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>0.39 wt%</td>
<td></td>
</tr>
<tr>
<td>Ca</td>
<td>4.34 wt%</td>
<td></td>
</tr>
<tr>
<td>Ti</td>
<td>0.58 wt%</td>
<td></td>
</tr>
<tr>
<td>Cr</td>
<td>0.20 wt%</td>
<td></td>
</tr>
<tr>
<td>Mn</td>
<td>0.23 wt%</td>
<td></td>
</tr>
<tr>
<td>Fe</td>
<td>12.87 wt%</td>
<td></td>
</tr>
<tr>
<td>Ni</td>
<td>0.05 wt%</td>
<td></td>
</tr>
<tr>
<td>Zn</td>
<td>0.03 wt%</td>
<td></td>
</tr>
<tr>
<td>Br</td>
<td>0.02 wt%</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. The Martian atmosphere and regolith composition used for the simulations.
For the DAN data analysis, the mass fractions, $\xi_A$, are assumed to correspond to the average regolith composition at Gusev and Meridiani measured by the APXS experiment on-board the NASA Mars Exploration Rovers (MERs) (see Tables 4.1 and 4.2 in [23]). Up to now, this is the most representative data published, which describes the regolith at a number of different locations of the MER traverses. Only a few publications are available regarding the regolith composition measurements performed by the rovers instruments at different Curiosity stops to this point. Moreover, all these instruments provide information about the regolith properties of a small spot on the surface or of a small mass sample, while DAN collects data from a large volume (~ 1.5 m radius × 60 cm in depth, see Section 4.6) of the regolith directly below the DAN instrument. Therefore, for the regolith composition, we will use the MER soil composition data for all elements, except hydrogen, oxygen and chlorine (see below). However, it is probable that in the future the regolith composition from MERs will be replaced by the data from the Curiosity measurements at Gale Crater.

Moderation of leaking neutrons is produced mainly by hydrogen nuclei, and assuming H in water, each atomic mass unit of H brings 8 atomic mass units of oxygen to the total mass balance of the soil. Therefore, we will use the mass fraction of water $\xi_W$, as the variable parameter for albedo neutron moderation.

The variable content of chlorine was proposed in Ref. [16] to take into account the variable absorption of thermal neutrons in the soil. However, it is known that chlorine is not the only element that has a large cross-section for the absorption of thermal neutrons (there is also iron, titanium, etc.). For making a DAN data analysis, one cannot vary all individual absorbing atoms. Instead, we use a single variable parameter, the content of absorption equivalent chlorine $\xi_{Cl}$, to take into account all absorbers of thermal neutrons (see Section 4.5 and [8,11]).

A list of the main rock-forming elements, $A$, with concentrations $C_A$ greater than 0.02 wt% is shown in Table 1. This composition is normalized to 100% without water and chlorine. The chlorine and water are not included in Table 1 because they are variable parameters in the analysis of regolith composition performed by the DAN team using the active measurements. To make the numerical model of the regolith, the concentrations of all elements, A, except hydrogen, oxygen and chlorine should be used, following $\xi_A = C_A/(1 - \xi_W - \xi_{Cl})$. The concentration of chlorine is $\xi_{Cl} \cdot 100\%$, the concentration of hydrogen, is $1/9 \cdot \xi_W \cdot 100\%$, and the concentration of oxygen, is $(8/9) \cdot \xi_W + (4/9) \cdot (1 - \xi_W - \xi_{Cl}) \cdot 100\%$.

To simulate by numerical modeling the variability of chlorine and other neutron absorbers from one rover stop to another, chlorine concentration $\xi_{Cl}$ variations from 0.5 to 1.7 wt% have been allowed. For regolith models with a fixed chlorine concentration $\xi_{Cl} = 1.0$ wt% has also been used. For the regolith density is a free parameter during initial modeling where it was allowed to vary from 1.2 to 2.5 g/cm$^3$. It was found that a regolith density of 1.8 g/cm$^3$ is a good approximation of the average regolith density at the first ~60 stops where DAN active measurements were performed [11]. Accordingly, the density of the regolith has been fixed at 1.8 g/cm$^3$ to reduce the number of free parameters in the regolith model.

4.5. The chlorine equivalent parameter, as neutron absorption parameter

The physics of introducing the absorption equivalent chlorine parameter follows. The average free path for neutron absorption $L_{ab}^{-1}$ is presented in Eq. (6):

$$L_{ab}^{-1} = n_A \cdot \sigma_A + n_W \cdot \sigma_W + \sum_A n_A \cdot \sigma_A$$

Eq. (8) helps to understand the physical sense of the parameter of absorption equivalent chlorine: it is equal to the actual content of chlorine $C_{Cl}$ plus/minus contributions due to the differences of fractions of other absorbing atoms from their standard values according to APXS MER. Provided the relative fractions of other absorbing elements are equal to the APXS MER values, $\xi_{Cl} = C_{Cl}$. Generally speaking, Eq. (8) may be considered as the empirical relationship between the unknown values of the abundances of chlorine and other neutron absorbing elements. It is based on the known values of $\xi_{Cl}$ and $\xi_W$, which were found from the DAN data analysis.

Initial studies (see [16]) have shown that, in addition to chlorine, there would be several other absorbers of thermal neutrons (such as isotopes of Fe, Mn, Ti, etc.), which could be taken into account for the interpretation of DAN measurements. Following a similar approach, we may transform Eq. (8) into a numerical formula by taking into account only major neutron absorbers. They could be determined using their thermal neutron capture cross-sections, the values of abundances and standard deviations of abundances according to the APXS MER data (see [23]). According to this approach, the three major contributing isotopes are $^{56}$Fe ($\xi_{56Fe} = 11.8 \pm 3.2$ wt%), $^{32}$S ($\xi_{32S} = 3.6 \pm 2.7$ wt%) and $^{48}$Ti ($\xi_{48Ti} = 0.4 \pm 0.2$ wt%). Keeping in Eq. (8) these three major additional members, one gets from this equation:

$$\xi_{Cl} = \frac{\sigma_{Cl}}{\rho \sigma_W \mu_W} + 1.01 \cdot (1 - \xi_W - \frac{\sigma_{Cl}}{\rho \sigma_W \mu_W}) \cdot \left[ 0.037 (\xi_{56Fe} - 0.118) + 0.013 (\xi_{32S} - 0.036) + 0.14 (\xi_{48Ti} - 0.004) \right]$$

(9)

It is evident from Eq. (9) that the chlorine absorption equivalent parameter, $\xi_{Cl}$, could be quite close to the actual value, $C_{Cl}$. Indeed, using the APXS values and measured standard deviations for the abundances of Fe, S and Ti for the corresponding differences $\xi_{Cl} - C_{Cl}$ (see Eqs. (8) and (9)), one finds the contributions of the measured uncertainty of these elements abundances to the deviation from $C_{Cl}$: 0.037 - 0.032 = 0.0012, 0.013 - 0.036 = 0.0004, 0.14 - 0.004 = 0.0003, respectively. For the expected chlorine content of about 0.01, these contributions produce small corrections of 12%, 4% and 3%, respectively. However, even for such a small possible difference
between the values of $\xi_{c1}$ and $\xi_{c2}$, we emphasize in the text below that our estimate for the chlorine abundance is based on the approximation of the absorption equivalent chlorine in Eq. (8).

4.6. Estimation of the DAN depth sensitivity to layer of water ice

For many purposes it is useful to understand the depth limit of the DAN sensitivity to the presence of water in the subsurface. This limit may be estimated by numerical modeling of active DAN measurements for a double-layer regolith with a dry top layer and pure water ice lower layer. Additionally, the sensitivity depth can be evaluated by the instrument ground calibrations.

Simulations have been performed for two-layer models of the subsurface with a pure water ice layer at depths from 5 to 300 cm below a dry layer of regolith with 1.7 wt% of water and a density of 1.8 g/cm$^3$. It was found that the instrument was not able to detect a layer of pure ice at a depth below about 60 cm. Therefore, the depth of 60 cm is used as the limit for probing for hydrogen/water in the subsurface.

A special program of DAN ground calibration was performed to obtain an experimental estimate of the instrument depth sensitivity to a layer of water ice. A double layer regolith structure was modeled for these measurements. The dry top layer of regolith was modeled by one or several layers of silicon bricks (with $\sim$ 2.5 wt% of water). A layer of water ice was modeled by polyethylene bricks (for which the atomic fractions of hydrogen are similar). Variations of the dry layer thickness were modeled by varying the number of silicon brick layers above the polyethylene. With thickness of the top dry layer increasing, the DAN sensitivity to the presence of polyethylene decreases and, at the depth of $\geq$ 60 cm, the shapes of the measured die-away time profiles became indistinguishable from the curves measured for the “no hydrogen” case. This method also provides about 60 cm as the value of the instrument depth sensitivity.

So, both methods for testing the DAN depth sensitivity, numerical simulation and physical measurements, provide similar results. Thus, a depth of 60 cm is accepted for DAN data analysis as the sensing scale of DAN active measurements.

4.7. Corrections of models for rover back-scattering

For numerical simulations, a model of the Curiosity rover is also necessary. Detailed information about the rover mechanical structures and chemical composition is unavailable, so the rover composition and geometry were estimated by a special iterative procedure [8,17]. During this procedure, numerical model predictions for some selected rover compositions and physical measurements were compared with the data of DAN active measurements during the MSL pre-launch tests at the Kennedy Space Center (ATLO tests). The concrete floor, walls and ceiling of the testing hall of KSC were modeled in accordance with the test facility geometry. The rover was modeled upside-down (Fig. 6) to reproduce the rover position during the tests. The rover’s main body was modeled by a block with dimensions 120 cm $\times$ 162 cm $\times$ 44 cm. All six wheels were also included in the model, as they were fixed in their position for space flight. One of them is located close to the DAN PNG and may produce additional scattering of neutrons, while another one is located close to the DAN DE and again may provide an additional scattering of neutrons to the detectors during active measurements. The rover’s robotic arm was not included in the numerical modeling because of its large distance from the DAN position on the opposite side of the main body of the rover.

The rover model includes a detailed model of the MMRTG—a nuclear power source for MSL. It generates electrical power utilizing the heat produced by the radioactive $\alpha$-decay of plutonium isotopes (primarily of $^{239}$Pu with half-life of 87.7 years) in the PuO$_2$ fuel. The MMRTG produces a continuous neutron flux with a broad energy spectrum. A detailed description of the MMRTG irradiation may be found in Ref. [17].

Since detailed information about the chemical composition of the MSL main mass distribution structure is not available, some typical compositions of the main block of spacecraft avionics and scientific instruments have been used as the starting point for the iterative modeling. Predicted time profiles of counts in CTN and CETN were compared with DAN testing data at KSC, and the difference between the simulation and measurements was evaluated. Then, the composition was iteratively changed within the known engineering limitations to find the best mass model of the rover that provides the best agreement with the measurements at KSC. This iteration procedure of modeling was finished, when a reasonable agreement was achieved between the ATLO-measured data and numerical simulations (Fig. 7). The final accepted mass model of the rover has a total mass of $\sim$ 920 kg and contains uniformly distributed material with density of 0.95 g/cm$^3$ and the following composition: 0.4 wt% of hydrogen, 3.2 wt% of carbon, 16.0 wt% of oxygen, 39.13 wt% of aluminum, 7.83 wt% of nitrogen, 31.30 wt% of titanium, 2.14 wt% of copper. This composition provides a better agreement between the ATLO-measured data and numerical simulations than the rover composition model used in Ref. [17] which is a two-compartment rover model, consisting of aluminum and polyethylene. It is easy to see from Fig. 7 that the numerical mass model of the rover is able to reproduce the main features of the measured DAN data at KSC, but there are still some areas for future improvements of the mass model, for example, the discrepancy between the measured data and simulated values in the time range $< 20$ $\mu$s after the pulse. However, the current mass model of the rover is used for the present analysis of the DAN active measurements (e.g. see [8,10,11]). We plan to update the rover model in the future, as we collect more active data from the surface operations.

The measured die-away time profiles of the CTN and CETN are mainly contributed by the albedo neutrons from the regolith, but they are also contributed by neutrons back-scattered from the material of the rover. Therefore, generally speaking, numerical simulations of neutron counting time profiles should be based on the combined model of the surrounding mass, which includes both the model of the regolith subsurface and also the mass model of the
rover. Such comprehensive modeling requires a large number of Monte Carlo computations, which allow comparisons of the measured time profiles of neutron albedo to the corresponding simulated curves. The Monte Carlo computations should be done for a large number of points within the space of the soil parameters. Since the rover mass models could be revised in the future, it is not practical to perform such a comprehensive numerical calculations for the mass distribution model, which includes the irradiated subsurface with the rover on top of it. Indeed, when the mass model of the rover is changed, the computations must be entirely repeated. Instead, in the current data analysis procedure, we postulated that one may take the rover mass into account by multiplying the time profiles \( F_{\text{meas}}(t_i) \) and \( F_{\text{mod}}(t_i) \) for the CTN and CETN detectors, which were simulated for the mass of the regolith only, by special time-dependent correction coefficients \( R_{\text{meas}}(t_i) \) and \( R_{\text{mod}}(t_i) \), which take into account the contributions of the rover:

\[
W_{\text{meas}}(t_i) = F_{\text{meas}}(t_i) \cdot R_{\text{meas}}(t_i)
\]

Therefore, there are time profiles, \( W_{\text{meas}}(t_i) \), which one should compare with the measured time profiles of thermal and epithermal neutrons. The coefficients \( R_{\text{meas}}(t_i) \) and \( R_{\text{mod}}(t_i) \) have been found from the numerical modeling of the DAN active measurements for the regolith with a typical mass composition with and without the presence of the rover’s body on the surface, \( W_{\text{mod}}(t_i) \) and \( F_{\text{mod}}(t_i) \), respectively. The coefficients \( R_{\text{meas}}(t_i) \) are the ratios of these time profiles, \( R_{\text{meas}}(t_i) = W_{\text{meas}}(t_i)/F_{\text{meas}}(t_i) \). They are obviously different for the CTN and CETN and vary with time following the DAN PNG pulse (see Fig. 8). Such an approach corresponds to the physical concept of accounting for the rover contribution as a neutral mirror of neutrons, which adds counts of leaking neutrons due to their back-scattering. Numerical modeling of the profiles \( W_{\text{meas}}(t_i) \) and \( F_{\text{meas}}(t_i) \) for a representative number of subsurface compositions has shown that, indeed, the variations of the coefficients \( R_{\text{meas}}(t_i) \) are rather small in comparison with the overall accuracy of the numerical modeling of neutron albedo. Therefore, we use this approach for the DAN data analysis, which helps to save significantly the computational time for the numerical during modeling. In the future, if the rover mass model is modified, it would be easy to change the correction factors accordingly, without recomputing the modeling time profiles of neutrons from the subsurface.

5. Data analysis of the DAN active measurements

5.1. Usage of DAN active data for testing regolith models

Since the real contribution of rover mass for neutron back-scattering is not known well enough, and due to some uncertainty in the instrument sensors’ absolute response functions, it is practically impossible to numerically simulate for any given soil an absolute values of neutron counting rate with high precision. At the same time, the relative variations of die-away curves may be modeled with high accuracy for different models. One may fit the measured data from a given Curiosity location using an amplitude-scaling factor as a free parameter. In this approach only the shape of die-away curves of modeled and measured signals are compared; the amplitude is excluded from the fitting procedure. This approach does not use properly all opportunities of the active neutron sensing because variations of neutron flux leakage from the Martian surface after the DAN PNG pulse are known to be strong parameters on the regolith composition. Therefore, another approach has been chosen: some particular reference testing spot is selected and amplitude scaling factors \( k_{\text{fl}} \) and \( k_{\text{etn}} \) are found for STN and SETN, which provide the best match between the measured and simulated counting rates for thermal and epithermal
neutrons, respectively. The reference spot should be selected by the condition that the properties of its soil could be fitted by some individual models for each group of tested models.

It was found that all tested regolith models are consistent with data gathered at the Curiosity stop at odometry 7.01 m (see Section 5.4); therefore, we have selected this point to estimate the amplitude scaling factors. We then fix scaling factors, $k_{\text{CTN}}$, and multiply the simulated values, $W_{\text{CTN}}(t)$, by these factors for all other locations to allow the direct comparison of amplitudes of simulated die-away time profiles with the observed curves.

It was found from numerical modeling that for die-away curves measured by the CTN and CETN detectors there are some intermediate time intervals after pulses, where the shape and the amplitude of the curves are mostly dependent on the hydrogen variation in the regolith. Indeed, in early time bins of the die-away curves the neutrons backscattered by the rover body are significantly greater than neutrons backscattered by regolith. On the other hand, in later time bins, neutrons from distant vicinity dominate in count rate. Regolith properties at these greater distances around the rover may be significantly different from the regolith properties closest to the instrument, and data could be biased by such variation. So, the later time bins of the die-away curves should be also better excluded from analysis.

Only middle time bins should be used in the data analysis to find regolith properties closest to DAN. Thus, for the CTN and CETN detectors, time intervals 478–1135 $\mu$s and 122–249 $\mu$s after the neutron pulse, respectively, have been selected (see Fig. 9). These intervals have been selected after analysis of a large set of DAN active measurements and a number of numerical simulations. It was found that variations of the measured signal at these intervals are the most sensitive for variations of the hydrogen concentration. This may be illustrated by comparing the measured die-away curves of thermal and epithermal neutrons for one of the driest and one of the wettest locations is presented in Fig. 9: the presence of hydrogen produces a higher and continuous thermal neutron albedo from the regolith at time $> 200 \mu$s after the neutron pulse and reduces the albedo of epithermal neutrons at 100–300 $\mu$s. It is important that, even in cases where wet regolith is covered by a dry layer, the thermal and epithermal neutron albedo demonstrates very visible features at times 100–2000 $\mu$s (see Fig. 10).

Also, the selected time intervals may be used for determination of chlorine concentration. Fig. 11 illustrates a comparison of die-away curves measured at spots with low and high chlorine abundance in the regolith. High chlorine abundance reduces thermal neutron albedo after 200 $\mu$s and only slightly reduces epithermal neutron albedo after $\sim 130 \mu$s.

**Fig. 9.** (a and b) Examples of die-away curves measured by the CTN (a) and CETN (b) during Curiosity stops at driest (red curves) and wettest (blue curves) sites. The time intervals selected for water concentration estimation are shown between dashed vertical lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

**Fig. 10.** (a and b) Examples of die-away curves measured by the CTN (a) and CETN (b) during Curiosity stops at a place with homogeneous (red curves) and at a place with strong double layered (blue curves) hydrogen distribution in the subsurface regolith. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
5.2. Testing the regolith models by DAN active data

To estimate regolith model parameters at a particular Curiosity stop where the DAN active measurements have been made, a comparison of measurements and numerical model predictions should be done using the data gathered at the selected time intervals. From a statistical point of view, it is necessary to test the hypothesis that measured die-away curves are consistent with numerical model predictions for a regolith with selected water concentration, $\xi_W$, and its distribution in the regolith, chlorine concentration, $\xi_C$, and regolith density, $\rho$. Quantitative tests of model and measurement consistency may be performed using the Pearson $\chi^2$ statistical criterion for the function:

$$S = \sum_{i=1}^{n} \left( \frac{A_{\text{meas}}(t_i) - k_{\text{meas}} \cdot W_{\text{meas}}(t_i)}{\sigma_{\text{meas}}(t_i)} \right)^2 + \sum_{k=1}^{m} \left( \frac{A_{\text{mod}}(t_k) - k_{\text{mod}} \cdot W_{\text{mod}}(t_k)}{\sigma_{\text{mod}}(t_k)} \right)^2,$$

(11)

where $A_{\text{meas}}(t_i)$ and $\sigma_{\text{meas}}(t_i)$ are the normalized measured count rates (see Eq. (4)) and statistical uncertainty of the measurement at time bin $t_i$ of a CTN and CETN detector’s die-away curve. The values $W_{\text{meas}}(t_i)$ and $\sigma_{\text{meas}}(t_i)$ are the counting rates and uncertainty (due to the Monte Carlo simulation process) in the same bin, $t_i$, predicted by numerical modeling for the selected regolith parameters. The time intervals selected in the previous section are used for this testing: for the thermal neutron detector, CTN, from $\varepsilon^{\text{ctn}}_1$ to $\varepsilon^{\text{ctn}}_n$, which corresponds to time interval 478–1135 $\mu$s after the neutron pulse and for the epithermal neutron detector, CETN, from $\varepsilon^{\text{ctn}}_1$ to $\varepsilon^{\text{ctn}}_n$, which corresponds to time interval 122–249 $\mu$s. These time intervals are completely covered by 12 bins on the DAN instrument time scale. Lastly, $k_{\text{meas}}$ and $k_{\text{mod}}$ are the amplitude scaling factors. If the regolith parameters are correct, the numerical predictions, $W_{\text{meas}}(t_i)$, are in agreement with measurements, $A_{\text{meas}}(t_i)$, within the uncertainties of modeling $\sigma_{\text{meas}}(t_i)$ and measurements $\sigma_{\text{meas}}(t_i)$ and each term at Eq. (11) have zero mean and $S$ achieves its minimum value.

If the difference between the measurements and the model is due to random fluctuations, the $S$ function has the $\chi^2_{\text{DOF}}$ distribution with degrees of freedom, $\text{DOF} = (\varepsilon_{\text{ctn}}^{\text{ctn}} - n) + (\varepsilon_{\text{ctn}}^{\text{ctn}} - 1) - \lambda$. The $\lambda$ here is the number of free parameters of the selected regolith model. Selection of the wrong parameters of the regolith model will introduce an additional contribution to $S$ from the systematic errors in the model $W_{\text{meas}}(t_i)$ providing $S$ large than expected. Therefore, a hypothesis that the selected parameters are correct is rejected at significance level $\alpha$ if $S$ is found to exceed the $\alpha$-point of the $\chi^2_{\text{DOF}}$ distribution, defined by

$$\alpha = \int_{\chi^2_{\text{DOF}}}^{\infty} f(y^2) \, dy^2,$$

(12)

where $f(y^2)$ is the probability density of the $y^2$ distribution. Rejection at significance level $\alpha = 1\%$ has been selected; this means a set of parameters must be rejected if $S > \chi^2_{\text{DOF}}(0.01) = \chi^2_{\text{DOF}}(0.01) = 20.09$ must be rejected with the confidence level of 1%.

5.3. Estimation of the regolith model parameter uncertainties

There are at least two methods to estimate the uncertainty of the best fitting model parameters that have been found by a procedure similar to that described in the previous section. One of these methods is a very reliable method suggested for X-ray astronomy by Lampton et al. [24]. This method suggests estimating uncertainty of a parameter in a tested regolith by estimating a region in parameter space which is located inside the boundary $S_{\lambda} = S_{\text{min}} + \chi^2_{\lambda} \alpha$, where $\lambda$ is a number of free parameters of the tested regolith model, $S_{\text{min}}$ is a value obtained from Eq. (11) for best fitting regolith model parameters and $\alpha$ is a confidence level of the parameters acceptance. Thus, for example, as described at the end of the previous section, for $\lambda = 4$ and for the “1σ” confidence level (68.27% confidence interval) one may calculate the $\chi^2(1 - 0.6827) = 4.719$. Therefore, the uncertainties of parameters at the “1σ” confidence level correspond to the $S_{\lambda}$ located inside the $S_{\text{min}} + 4.719$ volume in the parameters space.

However, this method has a significant difficulty for the task we’re considering. To find the boundary in the parameters space, $S_{\lambda}$, precisely, it is necessary to fill the parameter space with a wide grid of parameter values. This is a very time-consuming task since the necessary range of parameters is not known a priori, an optimal step of the grid is also unknown and, most importantly, the calculation of each $S$ in this grid requires Monte Carlo simulations of $W_{\text{meas}}(t_i)$ using the MCNPX code.

Taking into account this difficulty, a method of estimating the model parameter uncertainties based on Monte Carlo simulations was
introduced. This method is based on ideas described in Section 15.6 of [25]. These ideas may be implemented for DAN active data processing with some modification since searching for best-fit regolith model parameters is performed on a precalculated grid in parameter space with interpolation between nodes. Thus, the suggested method requires multiple Monte Carlo simulations of the measured die-away curves, \( A_{\text{in}}(t) \), according to the uncertainties of measurements, \( \sigma_{\text{in}}(t) \). Then the simulated data are used, as the measured data, in the standard process of the best regolith parameter estimation. Dispersion of obtained values for the parameters characterizes the uncertainty of their evaluation. It was found that it is sufficient to repeat this simulation 256 times to estimate the uncertainty of parameters with enough precision. The result of this simulation is a sample of 256 regolith parameters generated in the \( \lambda \)-dimensional parameter space. The standard deviation of this sample of each parameter is taken as the parameter uncertainty.

It was verified that both methods provide close estimates of uncertainties, but the first method requires a significantly large amount of MCNPX simulations. Therefore, the second method was selected as our baseline.

5.4. Example of the regolith model parameters estimation

Since water content is thought to be the parameter most likely responsible for the observed variations of neutron albedo at different spots where DAN active measurements were performed, four regolith model groups are introduced and tested for consistency with measurements to determine soil parameters (see [11] for details).

The simplest group, Model Group 1 (MG1) is introduced first. The MG1 is a group of models with a standard regolith composition (see Section 4.4), a fixed volume regolith density of 1.8 g/cm\(^3\), and a fixed content of 1 wt% for the absorption equivalent chlorine. Only one variable parameter is allowed for these MG1 models—the water content \( \xi_W \) over the 60 cm sensing depth of the DAN instrument. It was shown by Mitrofanov and co-authors [11] for the data at the initial part of 1900 m of the rover traverse that the MG1 is acceptable with probability \( a \geq 1\% \) for 40 different locations, which is only 26% of the entire suite of observations, along the first 1900 m of the Curiosity traverse. Therefore, while some models of MG1 might work for individual testing spots, the MG1 group with a single variable parameter (\( \xi_W \)) cannot explain the soil variations over the full set of active measurements at all locations.

The next level of model complexity is represented by the Model Group 2 (MG2). Models of this group, with a standard regolith composition, allow two variable parameters: soil density, \( \rho \), and water content, \( \xi_W \). In 52 cases (corresponding to 34% of testing spots along the first 1900 m of the Curiosity traverse), MG2 was able to fit the observations with a confidence higher than 1% [11]. Also, the MG2 group does not provide any significant change in the estimated water content parameters compared with them for MG1. Therefore, one may conclude that the inclusion of variable density alone does not improve the quality of data modeling.

The Model Group 3 (MG3) allows variable water content, \( \xi_W \), and absorption equivalent chlorine content, \( \xi_{\text{Cl}} \). This group is very important for data interpretation because the effect of neutron absorption by chemical elements like chlorine is known to change the time profile of post-pulse emission of thermal neutrons. Indeed, there are 87 testing spots for which the data are consistent with the best fit models of MG3, having an acceptance probability greater than 1%, which corresponds to 56% of testing spots along the first 1900 m of the Curiosity traverse. It is better than MG1 and MG2, but still not enough for acceptable data interpretation.

The next complex group, Model Group 4 (MG4), introduces two distinct water-bearing layers in the subsurface. One knows that the post-pulse time profile of neutron emission is rather sensitive to the vertical distribution of hydrogen and a two-layer model is the simplest approach to take this effect into account. So, the models of MG4 have two independent parameters of water content for top and bottom layers, \( \xi_W^{\text{top}} \) and \( \xi_W^{\text{bottom}} \), a third parameter is the thickness, \( h \), of the top layer and a fourth parameter is the content of absorption equivalent chlorine, \( \xi_{\text{Cl}} \). It was found that data for practically all testing spots are well fit by the two-layer models of MG4: 152 spots, or 99%, have acceptance level \( a \geq 1\% \) (see Table 2 in [11]). Therefore, the MG4 is selected for the DAN active data analysis and corresponding evaluations of soil parameters at tested spots along the traverse.

Examples of consistency between model groups and measurements are shown in Table 2. Acceptance probability values for model groups MG1–MG4 are considered for four different cases of DAN active measurements. The first row presents acceptance probability for MG1–MG4 tested with the DAN active data gathered during Sols 17–21 at the second Curiosity stop located about 7 m away from the Bradbury landing site. It is easy to see that all four model groups are able to provide statistically acceptable fits to the data at this site including the simplest one (MG1 group). This spot is used for estimating the amplitude scaling factors, \( k_{\text{in}} \) and \( k_{\text{em}} \) (see Section 5.1). The next rows of Table 2 illustrate more complicated cases of soil structure. So, the DAN active measurements at Sol 338 (odometry 1111.63 m) were done at a site, where soil structure cannot be fitted by any model of the simplest models MG1. This means that the standard regolith model with a variable water concentration is not enough to describe the subsurface observed at this location and additional variable parameters of a regolith model (such as variable concentration of chlorine or variable density) are required, which can be provided by using groups MG2–4. The next row (DAN measurements at Sol 494 at odometry 4623.00 m) illustrates even more strict requirements to the selection of regolith models. In this case, both MG1 and MG2 are not able to provide soil models consistent with measurements. At least two physical parameters of the regolith are required: variable water and chlorine content. Finally, the last row (DAN measurements at Sol 546 at odometry 5110.19 m) of Table 2 shows the most complicated case where the double-layered model (the MG4 group of models) with

<table>
<thead>
<tr>
<th>Sol Odometry, m</th>
<th>MG1 (%)</th>
<th>MG2 (%)</th>
<th>MG3 (%)</th>
<th>MG4 (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>17–21</td>
<td>36.55</td>
<td>73.01</td>
<td>42.02</td>
<td>86.65</td>
</tr>
<tr>
<td>338</td>
<td>0.00</td>
<td>22.39</td>
<td>44.21</td>
<td>79.71</td>
</tr>
<tr>
<td>494</td>
<td>0.00</td>
<td>0.36</td>
<td>27.43</td>
<td>99.57</td>
</tr>
<tr>
<td>546</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>97.22</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Probability (%)</th>
<th>( \xi_W^{\text{top}} ) (wt%)</th>
<th>( \xi_W^{\text{bottom}} ) (wt%)</th>
<th>h (cm)</th>
<th>( \xi_{\text{Cl}} ) (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>17–21</td>
<td>1.70 ± 0.18</td>
<td>1.10 ± 0.08</td>
<td>7 ± 9</td>
<td>1.10 ± 0.08</td>
</tr>
<tr>
<td>338</td>
<td>1.70 ± 0.31</td>
<td>2.80 ± 0.64</td>
<td>20 ± 7</td>
<td>1.30 ± 0.16</td>
</tr>
<tr>
<td>494</td>
<td>1.50 ± 0.38</td>
<td>3.20 ± 0.94</td>
<td>30 ± 7</td>
<td>1.78 ± 0.18</td>
</tr>
<tr>
<td>546</td>
<td>1.70 ± 0.35</td>
<td>4.70 ± 0.97</td>
<td>26 ± 5</td>
<td>1.90 ± 0.11</td>
</tr>
</tbody>
</table>
variable water in the top and bottom layers of the regolith, a variable thickness of the top layer and variable content of chlorine is the only choice to get good agreement between observations and model predictions.

6. DAN data products for active measurements

Currently, DAN team provides the five following data products to the Planetary Data System (PDS):

1. Engineering data—contains the DAN instrument housekeeping parameters: time, temperatures, high-voltage (HV) levels, discriminator settings, local solar time.

2. Derived passive data (time series)—contains data frames collected by the DAN in the passive mode: time of measurements, coordinates of the rover at start and stop of data collection, duration of data collection, measured counts and background values for the CTN and CETN detectors and local solar time. The DAN data are corrected for detectors efficiency by:

\[
C_{\text{corrected}}(t) = \frac{C(t)}{1 - e^{-a_1(t - a_2)}}
\]

where \(C(t)\) is measured count rate at time \(t\), \(a_1\) and \(a_2\) are constants derived from calibration measurements for each detector separately.

3. Derived active data (time series)—contains data frames collected by the DAN in active mode: time of measurements, coordinates of the rover at start and stop of data collection, duration of data collection, number of pulses per data frame, DAN PNG frequency (Hz), the instrument time scale (64 time bins), measured counts and background values for the CTN and CETN detectors, local solar time.

4. Averaged passive data (averaged over a location)—contains data frames collected by the DAN in the passive mode averaged by the MSL stops: time of measurements, coordinates of the current rover stop where data are collected, duration of data collection at the current rover stop, averaged counts as a sum of all counts normalized by Eq. \(13\) in all passive frames of the current location divided by the collection duration, statistical uncertainty (error) of averaged counts, background values for the CTN and CETN detectors, local solar time.

5. Averaged active data (averaged over a location)—contains data frames collected by the DAN in the active mode averaged along the MSL stops and along measurements with the same instrument time scale: time of measurements, coordinates of the current rover stop where data are collected, duration of data collection as a sum of all collection duration values of the frames in the current location, number of pulses as a sum of all pulses across the frames of the current average set, DAN PNG frequency (Hz), time bins start and stop times for current time scale, averaged counts for the CTN and CETN detectors as a total number of counts in current bin across all active frames of the current location divided by the number of pulses (sum in all frames of the location) divided by the current time bin duration in seconds, statistical uncertainty (error) of averaged counts as the square roots of the total number of counts in current bin across all active frames of the current location and then divided by the number of pulses (sum in all frames of location) divided by the time bin duration in seconds, the total number of pulses across all frames in current location, start and stop local solar time of the averaged measurement.

7. Conclusion

This paper presents a detailed description of the DAN data processing procedure starting from the initial level of raw measurements up to the level of model-dependent deconvolution of various regolith properties along the Curiosity traverse. It is shown that this procedure can be used to determine such Martian regolith parameters as average density, chlorine equivalent concentration and hydrogen distribution. The regolith model parameters derived through this approach have successfully fit about 99% of sites where DAN active measurements have been acquired. In this paper we have focused on the details of DAN data processing. Additional science discussion and interpretation are also presented in [8, 11].

Acknowledgments

The DAN team is thankful to the highly professional MSL project team members who have maximized opportunities for DAN measurements on Mars. The DAN team very much appreciates the work of colleagues from the N.L. Dukhov Institute for Automation for the development of the reliable PNG for this experiment. Also, the DAN team appreciates the valuable cooperative support of two national space agencies, Roscosmos and NASA, which, working together, have made this Russian-contributed instrument possible on an United States rover. Finally, the team thanks the Curiosity science community, which provided essential comments and advice to the DAN team during numerous discussions.

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References