Hydrol. Earth Syst. Sci. Discuss., 10, 1097–1125, 2013
www.hydrol-earth-syst-sci-discuss.net/10/1097/2013/
doi:10.5194/hessd-10-1097-2013

Hydrology and Earth System Sciences Discussions

The COsmic-ray Soil Moisture Interaction Code (COSMIC) for use in data assimilation

J. Shuttleworth[1,2], R. Rosolem[1], M. Zreda[1], and T. Franz[1]

[1]Department of Hydrology and Water Resources, University of Arizona, USA
[2]Department of Atmospheric Science, University of Arizona, USA

Received: 18 December 2012 – Accepted: 9 January 2013 – Published: 24 January 2013

Correspondence to: J. Shuttleworth (shuttle@email.arizona.edu)

Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

Soil moisture status in land surface models (LSMs) can be updated by assimilating cosmic-ray neutron intensity measured in air above the surface. This requires a fast and accurate model to calculate the neutron intensity from the profiles of soil moisture modeled by the LSM. The existing Monte Carlo N-Particle eXtended (MCNPX) model is sufficiently accurate but too slow to be practical in the context of data assimilation. Consequently an alternative and efficient model is needed which can be calibrated accurately to reproduce the calculations made by MCNPX and used to substitute for MCNPX during data assimilation. This paper describes the construction and calibration of such a model, COSMIC, which is simple, physically-based and analytic and, because it runs at least 50 000 times faster than MCNPX, is appropriate in data assimilation applications. The model includes simple descriptions of (a) degradation of the incoming high energy neutron flux with soil depth, (b) creation of fast neutrons at each depth in the soil, and (c) scattering of the resulting fast neutrons before they reach the soil surface, all of which processes may have parameterized dependency on the chemistry and moisture content of the soil. The site-to-site variability in the parameters used in COSMIC is explored for 42 sample sites in the COsmic-ray Soil Moisture Observing System (COSMOS), and the comparative performance of COSMIC relative to MCNPX when applied to represent interactions between cosmic-ray neutrons and moist soilis explored. At an example site in Arizona, fast neutron counts calculated by COSMIC from the average soil moisture profile given by an independent network of point measurements in the COSMOS probe footprint are similar to the fast neutron intensity measured by the COSMOS probe. Moreover at this site application of data assimilation using COSMIC to update the Noah Land Surface Model constrains the modeled soil moisture such that it agrees with the values given by the independent network of point measurements, thus confirming that COSMIC can be used as a robust forward operator in data assimilation of cosmic-ray soil moisture measurements.

1 Introduction

Until recently area-average soil moisture at the hectometer horizontal scale has been difficult and costly to measure because of the need to take many point samples but with the advent of the cosmic-ray method (Zreda et al., 2008, 2012; Desilets et al., 2010) it is now feasible with a single instrument. However, a complicating aspect of measuring soil moisture using this method is that the volume of soil measured in the vertical varies with soil moisture content (Franz et al., 2012a).

One potentially important use of area-average soil moisture measured with the cosmic-ray method is through data assimilation methods to update the value of soil moisture states represented in the LSMs which are used to describe surface-atmosphere exchanges in meteorological and hydrological models. Typically such LSMs calculate (among many other things) time varying estimates of soil moisture content in discrete layers of soil defined within the vertical soil profile. In order to make use of the area-average soil moisture provided by the cosmic-ray method, it is necessary to:

1. diagnose if there is a discrepancy in the modeled soil moisture status from the above-ground measured fast neutron count; and
2. interpret knowledge of the extent of any discrepancy back into the LSM with weighting between layers reflecting their relative influence on the above-ground measured fast neutron count.

This requires the availability and use of an accurate model to interpret the modeled soil moisture profiles in terms of the above-ground fast neutron count.

In principle the required model needed to make such interpretation exists, specifically the Monte Carlo N-Particle eXtended (MCNPX: Pelowitz, 2005) neutron transport code, which was much used in establishing the cosmic-ray method (Zreda et al., 2008, 2012; Desilets et al., 2010) currently being deployed in the COsmic-ray Soil Moisture Observing System (COSMOS: http://cosmos.hwr.arizona.edu/; Shuttleworth et al., 2010;

Zreda et al., 2011, 2012). Given the specified chemistry of the atmosphere and soil (including the amount of hydrogen present as water in the system), the MCNPX code uses knowledge of nuclear collisions and libraries of nuclear properties for these constituents to track the life history of individual, randomly-generated, incoming cosmic rays and their collision products through the atmosphere and in the soil. The code then counts the resulting fast neutrons (we use those in the range 10 eV to 100 eV) that enter a defined detector volume above the ground. In principle the MCNPX code could be used in data assimilation applications to define (a) and (b) in the last paragraph. However, although accurate, the MCNPX code uses the time consuming Monte Carlo computational method and this means its use in data assimilation applications is impractical.

Therefore an alternative model is needed which can efficiently reproduce the below ground physics, the resulting above ground count rate and the below ground vertical source distribution of fast neutrons simulated by MCNPX. This paper describes the construction and calibration of such a model, the COsmic-ray Soil Moisture Interaction Code (COSMIC), which is simple, physically-based and analytic, and which runs much faster than MCNPX because the nuclear processes and collision cross sections that are explicitly represented in MCNPX are re-captured in parameters that have dependency on the site-specific soil properties. These parameters are calibrated using multi-parameter optimization techniques against MCNPX calculations for a suite of hypothetical soil moisture profiles.

2 Physical processes represented in COSMIC

The COSMIC model assumes there are three dominant processes involved in generating the fast neutrons detected above moist soil (see Fig. 1). It is first assumed that that there is an exponential reduction with depth in the number of the high energy neutrons that are available to create fast neutrons at any level in the soil. There is reduction due to interaction with both the (dry) soil and with the water that is present in the soil. The

HESSD
10, 1097–1125, 2013

exponential reduction therefore depends on two length constants L_1 and L_2, in units of gm per unit area, corresponding to interaction with the soil and the water (hydrogen), respectively. The mass of water includes both lattice water, i.e. that which is in the mineral grains and bound chemically with soil and considered fixed in time, and the pore water which is available to support transpiration or drainage and which consequently changes with time. Thus, the number of high energy neutrons available at depth z in the soil is given by:

$$N_{\mathrm{he}}(z) = N_{\mathrm{he}}^{0} \exp\left(-\left[\frac{m_{\mathrm{s}}(z)}{L_1} + \frac{m_{\mathrm{w}}(z)}{L_2}\right]\right) \quad (1)$$

where N_{he}^{0} is the number of high energy neutrons at the soil surface, $m_{\mathrm{s}}(z)$ and $m_{\mathrm{w}}(z)$ are respectively the integrated mass per unit area of dry soil and water (in gm per unit area) between the depth z and the soil surface, and L_1 and L_2 (in gm per unit area) are respectively determined by the chemistry of the soil and its total water content, including any chemically-bound lattice water.

Second, it is assumed that at each depth z the number of fast neutrons created in the soil is proportional to the product of the number of high energy neutrons available at that depth with the local density of dry soil and the local density of water at that depth, assuming the relative efficiency of creation of fast neutrons by soil is a factor α of the efficiency of their creation by water. Consequently, the number of fast neutrons created in the soil in the plane at level z is given by:

$$N_{\mathrm{f}}(z) = \left(CN_{\mathrm{he}}^{0}\right)\left[\alpha\rho_{\mathrm{s}}(z) + \rho_{\mathrm{w}}(z)\right] \exp\left(-\left[\frac{m_{\mathrm{s}}(z)}{L_1} + \frac{m_{\mathrm{w}}(z)}{L_2}\right]\right) \quad (2)$$

where C is a (unitless) "fast neutron creation" constant for pure water, $\rho_{\mathrm{s}}(z)$ is the local bulk density of dry soil and $\rho_{\mathrm{w}}(z)$ the total water content, including lattice water. It is assumed that the direction in which the fast neutrons are generated at level z is isotropic, i.e. that they leave with equal probability in all directions.

HESSD

10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

Finally it is assumed that the fraction of fast neutrons originating in the soil in the plane at level z that are detected above the ground are reduced exponentially by an amount related to the distance traveled between the point of origin in this plane and the detector at the surface. There is then little reduction in the neutron count in the air between the soil surface and the fast neutron detector mounted just a few meters above the surface. The reduction in fast neutrons in the moist soil is assumed to follow a functional form similar to that in Eq. (1) but with different length constants L_3 and L_4, in units of gm per unit area, corresponding to attenuation by soil and by (total) soil water, respectively. However, because the direction in which fast neutrons are generated at level z is assumed to be isotropic, fast neutrons reaching the surface will travel further if they do not originate directly below the detector, rather from a point that is more distant in the horizontal plane at level z. To allow for this it is necessary to calculate the integrated average of the attenuation for all points in this plane to the detector, with the attenuation distance being inversely proportional to $\cos(\theta)$ where θ is the angle between the vertical below the detector and the line between the detector and each point in the plane, see Fig. 2. Consequently, the integrated average attenuation of the fast neutrons generated at level z before they reach the detector is given by the function $A(z)$, thus:

$$A(z) = \left(\frac{1}{2\pi}\right) \int_0^{2\pi} \left[\left(\frac{2}{\pi}\right) \int_0^{\pi/2} \exp\left(\frac{-1}{\cos(\theta)} \left[\frac{m_s(z)}{L_3} + \frac{m_w(z)}{L_4}\right]\right) d\theta \right] d\phi \tag{3}$$

which, because there is assumed symmetry around the vertical through the detector, reduces to:

$$A(z) = \left(\frac{2}{\pi}\right) \int_0^{\pi/2} \exp\left(\frac{-1}{\cos(\theta)} \left[\frac{m_s(z)}{L_3} + \frac{m_w(z)}{L_4}\right]\right) d\theta \tag{4}$$

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

HESSD

10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

The value of $A(z)$ can be found numerically but for efficiency it could also be adequately calculated using the approach described in Appendix A.

Combining the representations of the three physical processes considered in COSMIC described above, the analytic function describing, N_{COSMOS}, the number of fast neutrons reaching the COSMOS probe at a near-surface measurement point is:

$$N_{\mathrm{COSMOS}} = N \int_0^\infty \left\{ A(z) \left[\alpha \rho_s(z) + \rho_w(z) \right] \exp\left(- \left[\frac{m_s(z)}{L_1} + \frac{m_w(z)}{L_2} \right] \right) \right\} \mathrm{d}z \tag{5}$$

Note that in Eq. (5), the product of the two constants (CN_o) that appears in Eq. (2) has been replaced by a single constant, N, because the values of C and N_o cannot be separately determined from a comparison between calculations made using COSMIC and MCNPX.

3 Determining the parameters to be used in COSMIC

To determine the values of the (in some cases site-specific) parameters to be used in COSMIC, at 42 selected sites in the COSMOS network (see Fig. 3) for which the required data were available at the time of this analysis simulations using COSMIC were calibrated against equivalent calculations made with the MCNPX model. The MCNPX calculations were made using the site-specific COSMOS probe calibration based on gravimetric samples (see, for example, Franz et al., 2012b), corrected for the effect of atmospheric humidity (see Rosolem et al., 2012), and with site-specific specification of soil chemistry and lattice water content.

The value of L_1 is easily determined for each site by running MCNPX with dry soil that has the site-specific soil chemistry and then fitting an exponential function to the calculated exponential reduction in high energy neutrons with depth simulated by MCNPX. Although the value of L_1 may depend on the soil chemistry present, our simulations with MCNPX at the 42 COSMOS sites considered in this study suggest that L_1 is only

HESSD
10, 1097–1125, 2013

weakly related to soil chemistry with site-to-site variability around the mean value for all sites being just $\sim 1\,\%$. On this basis, adopting a fixed value equal to $162.0\,\mathrm{g\,cm^{-2}}$ irrespective of site is a reasonable assumption.

Because L_2 and L_4 relate to attenuation by water alone, their values are independent of the soil chemistry of the site and they can be determined by substituting pure water for dry soil in MCNPX and COSMIC calculations. This determination was made at the original San Pedro site. A site-specific value of N was first determined for COSMIC at this site using a multi-parameter optimization of N, α and L_4 (similar to that described below but with the observed COSMOS count at the time of site calibration used when calculating the objective function rather than the equivalent count scaled from MCNPX). An exponential function was fitted to the calculated reduction in high energy neutrons with depth calculated by MCNPX for pure water to determine L_2 (analogous to the method used to determine L_1). The value of L_4 was then selected such that the COSMOS probe fast neutron count when calculated in the pure water simulations at the San Pedro site by MCNPX and by COSMIC (with the site-specific value of N) are equal. Based on these pure water simulation comparisons, the values of L_2 and L_4 were set to 129.1 and $3.81\,\mathrm{g\,cm^{-2}}$ at all COSMOS sites.

The values of the site-specific constants N, α and L_3 at all sites were then determined using multi-parameter optimization techniques against calculations made using MCNPX. At each site calculations of the above-ground fast neutron count are made using MCNPX for the 22 hypothetical profiles of volumetric water content illustrated in Fig. 4, i.e. for 10 profiles with different uniform volumetric water content, and 12 with different linear gradients of volumetric water content to a depth of 1 m and with uniform volumetric water content below 1 m. One criterion used in parameter optimization to define the preferred values of N, α and L_3 is the weighted Mean Absolute Error (MAE) between the above-ground fast neutron counts calculated using the COSMIC model and the equivalent counts calculated by MCNPX with the same profiles. In each case the MAE (i.e. COSMIC neutron flux minus MCNPX neutron flux for each profile in absolute terms) is weighted by the probability density function of soil moisture historically observed at each site, with the most commonly observed soil moisture values weighted to be twice as important as the least commonly observed value. The second criterion used in the optimization was that the cumulative contribution to above-ground fast neutrons as a function of depth given by the COSMIC model matches that calculated by MCNPX as reported by Zreda et al. (2008), i.e. at the site the cumulative contribution has a 2-e folding depth of around 0.76 m for a prescribed uniform volumetric water content of 0 %, and around 0.12 m for a prescribed uniform volumetric water content of 40 %.

The Multi-Algorithm Genetically Adaptive Multi-objective (AMALGAM) method (Vrugt and Robinson, 2007) was used to solve this multi-criteria minimization problem. AMALGAM contains highly desirable features for model optimization which facilitate parameter convergence, such as the use of multi-operator search and self-adaptive offspring creation, as well as the implementation of population-based elitism search. The initial parent population of size n is generated using Latin Hypercube Sampling (McKay et al., 1979). The Fast Non-dominated Sorting algorithm approach (Deb et al., 2002) is used to assign the Pareto-rank for multiple criteria. Subsequent generation of the offspring (with the same size n) occurs with the use of k operators. The approach adopted in this study, which is similar to that presented by Rosolem et al. (2012), uses a population of size $n = 100$, and number of operators (search strategies) $k = 4$, and set the maximum number of generations, $s = 1000$, so that the total number of simulations ($s \times n$) is 100 000.

This multi-parameter optimization was made at all 42 sites considered in this study to obtain the site-specific preferred values of N, α, and L_3 when the values of L_1, L_2 and L_4 are specified to be 162.0, 129.1 and 3.81 $\mathrm{g\,m\,cm^{-2}}$, respectively. The resulting optimal parameters are given in Table 1 (The factor F given in column four of this table is discussed and used later in Sect. 5). Figure 5 summarizes the overall results of the multi-parameter optimization procedure. In this figure the value of the difference between the simulated neutron count given by COSMIC (with optimized parameters) and the equivalent neutron count scaled from MCNPX, normalized by the MCNPX count, is

HESSD
10, 1097–1125, 2013

represented by colors for each site and each hypothetical soil moisture profile. Because MCNPX is a Monte Carlo model the neutron count given by MCNPX is subject to random sampling errors of the order 1 %, and this contributes to some of the normalized differences illustrated in Fig. 5. For a substantial majority of the sites and hypothetical soil moisture profiles the normalized difference between the COSMIC and MCNPX simulated neutron counts is within the range 2–3 % and when averaged over all sites the normalized difference is much less than this. This range in normalized difference is comparable to the measurement uncertainty in the COSMOS probe and the sampling error in the soil moisture field at probe calibration. However for very dry profiles the normalized difference is greater but still comparable to the range of uncertainty of the COSMOS probe.

4 Correlations and dependencies of optimized parameters

It is of interest to investigate the extent to which the site-specific optimized values of N, α and L_3 are correlated with each other and with the site-specific values of ρ_s, the average bulk density for the soil in gm cm^{-3}, and θ_{lattice}, the lattice water content of the soil in m^3 m^{-3}. In practice, there is no evidence of correlation between the site-specific value of the parameter N and the site-specific values of ρ_s, α and L_3: linear correlation of these three parameters with N gives R^2 values of 0.00, 0.14, and 0.00, respectively. There is also no evidence of correlation between the site-specific optimized values of α with θ_{lattice} at each site ($R^2 = 0.02$), and little evidence of correlation of N and L_3 with θ_{lattice} ($R^2 = 0.20$ and 0.14, respectively). However as Fig. 6 shows, the site-specific values of L_3 and α both exhibit evidence of correlation with ρ_s, the bulk density for the soil at each site, and the site-specific values of α and L_3 are also mutually correlated. Arguably L_3 and α are indeed both independently correlated with ρ_s, but the possibility exists that one of the parameters (likely L_3) is correlated and the apparent correlation of the second parameter (α), is because the process of optimization is not able to

HESSD
10, 1097–1125, 2013

clearly separate these two variables because their influence on N_{COSMOS} calculated by Eqs. (3) and (5) is to change its value in opposite directions.

It is worth noting that, in physical terms, a strong correlation between L_3 and ρ_s implies the attenuation of fast neutrons by (dry) soil is not well described as an exponential decay with a simple single length constant that is independent of the density of soil as assumed in COSMIC. Instead the effective value of the length constant appears to be a near-linear function of soil density. Similarly a (true) correlation between α and ρ_s implies that the creation of fast neutron from high neutrons is not perfectly described as a linear function of the local density of dry soil, i.e. in Eq. (2) the product $(\alpha\rho_s)$ becomes $(0.405(\rho_s)–0.102(\rho_s)^2)$. It is possible that the observed correlations of L_3 and α with ρ_s may be useful for COSMOS sites where a multi-parameter optimization against MCNPX is not feasible because approximate estimates of L_3 and α might then be made from measured value of ρ_s using the equations:

$$L_3 = -31.76 + 99.38\rho_s \tag{6}$$

$$\alpha = 0.405 - 0.102\rho_s \tag{7}$$

The marked variability in the site-specific optimized values of the parameter N must reflect substantial variability in one or both of the component constants C or N_{he}^0. However, there should be limited variability in N_{he}^0 because the site-specific neutron calculations given by MCNPX against which calibration was made were corrected for local station effects using a scaling factor to account for differences in cosmic ray intensity as a result of the elevation/cutoff rigidity of the site where the probe is located (for details see Desilets and Zreda, 2003). The contributing variability is therefore presumably primarily associated with the effective value of C. This site to site variability is intrinsic to the COSMOS array (rather than a feature associated with the COSMIC model) and is present in the site-specific factor F (given in column 4 of Table 1). F is the ratio between the number of counts observed during COSMOS probe calibration at a specific site and the calculated neutron flux intensity given by MCNPX when run with the soil chemistry and water content (including lattice water) observed at each probe site

HESSD
10, 1097–1125, 2013

during calibration. (Note: the factor 10^{14} in F arises because MCNPX actually calculates neutron fluence, the time integration of neutron flux, rather than neutron count rate directly.) Fig. 7 shows the strong interrelationship between the COSMIC parameter N found by multi-parameter optimization and the factor F which is:

$$N = -25.02 + 63.16 \cdot 10^{-14} F \tag{8}$$

The origin of the real site-to-site variability in F across the COSMOS array is currently under investigation. It is possible there is some remnant contribution to variability in F associated with the location and altitude of the probe although the neutron count rates were corrected for these (Desilets and Zreda, 2003). It is also possible that differences in the ambient water vapor content of the air during probe calibration may make some contribution to the variability in F at the level of a few percent (for details, see Rosolem et al., 2012). Otherwise the variability in F is presumably associated with site-to-site differences in soil chemistry or more likely vegetation cover (Franz et al., 2012b).

5 Application of the COSMOS probe at the Santa Rita study site

We tested COSMIC using soil moisture data from a COSMOS probe and from a distributed sensors network at the Santa Rita Experimental Reserve field site in southern Arizona. 180 Time Domain Transmissivity (TDT) sensors (Fig. 8a) were installed in 18 paired profiles at 10, 20, 30, 50 and 70 cm within the footprint of the COSMOS probe (Fig. 8b) (Franz, 2012c). Figure 8c shows a comparison between the fast neutron count observed by the COSMOS probe and that calculated from the area-average soil moisture as measured with TDT sensors using MCNPX and COSMIC. Overall the COSMIC derived fast neutron intensity compares quite well with measurements from the COSMOS probe and (as should be expected) it compares extremely well with thefast neutron intensity computed using MCNPX. In some cases, the after-rainfall response is slower than the COSMOS probe because the area-average soil moisture calculated

HESSD
10, 1097–1125, 2013

from TDT point sensors does not sample the near surface soil moisture above 10 cm depth and, as a result, does not recognize the faster rate of wetting and drying of surface soil moisture. Consequently, when the area-average profile measured by the TDT probes is used in the COSMIC model to calculate the COSMOS probe count, the estimated COSMOS count differs.

We applied the COSMIC model to assimilate COSMOS probe data into the Noah Land Surface Model (Koren et al., 1999; Chen and Dudhia, 2001; Ek et al., 2003) at the Santa Rita field site for a period during the North American Monsoon when there were rainstorms that generated rapid changes in soil moisture, see Fig. 9. In this figure the blue line shows the modeled depth-average soil moisture calculated by Noah without assimilation of COSMOS data, the red line shows the modeled depth-average soil moisture calculated by Noah with assimilation of COSMOS data, while the green line shows the depth-average soil moisture measured by the TDT network. To enhance consistency between these three depth averages they are all weighted by the relative contribution to the above ground fast neutron flux for each level (calculated by COSMIC). The Level 3 soil moisture provided on the COSMOS website for this period and site is also shown in black in Fig. 9, together with an estimate of the error in this value (shown in grey) that allows both for neutron counting statistics and estimated error in the calibration function. The improved consistency between modeled soil moisture and observations when COSMOS data is assimilated into Noah using COSMIC is clearly demonstrated by this figure, and by Table 2 which documents criteria that characterize the comparison between the different time series. On the basis of this table the remaining difference between observations and the model-derived depth-average soil moisture after assimilating COSMOS neutron counts is similar to the uncertainty between the two (TDT and COSMOS) observations.

HESSD
10, 1097–1125, 2013

6 Summary and conclusions

This study showed that COSMIC, a simple, physically based analytic model, can substitute for the time consuming MCNPX model in data assimilation applications, and that COSMIC can be calibrated by multi-parameter optimization at 42 COSMOS sites to provide calculated neutron fluxes which are within a few percent of those given by the MCNPX model. The three site-specific parameters defined by optimization are largely uncorrelated with each other, but two parameters, α and L_3, are correlated with ρ_s, the bulk density for the soil at each site, and consequently are mutually correlated. This correlation with ρ_s might provide an approximate estimate of their value if parameter optimization against MCNPX model is not feasible. The value of N, the third optimized parameter in COSMIC is very strongly related to F, i.e. to the ratio between the number of counts observed during COSMOS probe calibration at a specific site and the calculated neutron fluence given by MCNPX when run with the soil chemistry and water content (including lattice water) observed at each probe site during calibration. The origin of this real site-to-site variability in F across the COSMOS sensor array, which is presumably mainly associated with site-to-site differences in soil chemistry or more likely vegetation cover is currently under investigation. It was demonstrated that the calibrated COSMIC model with optimized site-specific parameters when applied at the Santa Rita Experimental Reserve field site to assimilate COSMOS probe counts into the Community Noah Land Surface Model effectively holds the weighted depth-average soil moisture simulated by the Noah model on track.

HESSD
10, 1097–1125, 2013

Appendix A

Integration of fast neutron attenuation over angles of emission

Calculation of the above-ground fast neutron detection rate by the COSMOS probe detector requires evaluation of the integral, $A(z)$, where:

$$A(z) = \left(\frac{2}{\pi}\right) \int_0^{\pi/2} \exp\left(\frac{-1}{\cos(\theta)}\left[\frac{m_s(z)}{L_3} + \frac{m_w(z)}{L_4}\right]\right) d\theta \quad \text{(A1)}$$

This integral can be re-written more simply as:

$$A(z) = \left(\frac{2}{\pi}\right) \int_0^{\pi/2} \exp\left(\frac{-x}{\cos(\theta)}\right) d\theta \quad \text{(A2)}$$

where x lies in the range zero to infinity and is defined to be:

$$x = \left[\frac{m_s(z)}{L_3} + \frac{m_w(z)}{L_4}\right] \quad \text{(A3)}$$

Equation (A2) can be evaluated numerically for any value of x but to speed calculations when using COSMIC in data assimilation applications, it can alternatively be calculated with accuracy better than one part in a thousand by expressing A analytically in the form:

$$A(z) = e^{y} \quad \text{(A4)}$$

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

HESSD

10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

and the function y calculated from x using functions that are defined for different ranges of x as follows:

for: $x \leq 0.05 \quad y = -347.86105x^3 + 41.64233x^2 - 4.018x - 0.00018$ (A5)

for: $0.05 < x \leq 0.1 \quad y = -16.24066x^3 + 6.64468x^2 - 2.82003x - 0.01389$ (A6)

for: $0.1 < x \leq 0.5 \quad y = -0.95245x^3 + 1.44751x^2 - 2.18933x - 0.04034$ (A7)

for: $0.5 < x \leq 1 \quad y = -0.09781x^3 + 0.36907x^2 - 1.72912x - 0.10761$ (A8)

for: $1 < x \leq 5 \quad y = -0.00416x^3 + 0.05808x^2 - 1.361482x - 0.25822$ (A9)

for: $5 < x \quad y = +0.00061x^2 - 1.04847x - 0.96617$ (A10)

Acknowledgements. The COSMOS project is funded by the Atmospheric Science, Hydrology, and Ecology Programs of the US National Science Foundation (grant ATM-0838491). We thank those who contributed in various ways to the COSMOS project and this paper, especially Xubin Zeng, Ty Ferre and Bobby Chrisman.

References

Chen, F. and Dudhia, J.: Coupling an advanced land surface-hydrology model with the penn state-NCAR MM5 modeling system. Part I: Model implementation and sensitivity, Mon. Weather Rev., 129, 569–585, 2001.

Desilets, D. and Zreda, M.: Spatial and temporal distribution of secondary cosmic-ray nucleon intensities and applications to in-situ cosmogenic dating, Earth Planet. Sci. Lett., 206, 21–42, doi:10.1016/S0012-821X(02)01088-9, 2003.

Desilets, D., Zreda, M., and Ferre, T.: Nature's neutron probe: land-surface hydrology at an elusive scale with cosmic rays, Water Resour. Res., 46, W011505, doi:10.1029/2009WR008726, 2010.

Ek, M. B., Mitchell, K. E., Lin, Y., Rogers, E., Grummann, P., Koren, V., Gayno, G., and Tarpley, J. D.: Implementation of Noah land surface model advances in the National Centers for Environmental Prediction operational Mesoscale Eta Model, J. Geophys. Res., 108, 8851, doi:10.1029/2002JD003296, 2003.

HESSD

10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

Franz, T. E., Zreda, M., Ferre, P. A., Rosolem, R., Zweck, C., Stillman, S., Zeng, X., and Shuttleworth, W. J.: Measurement depth of the cosmic-ray soil moisture probe affected by hydrogen from various sources, Water Resour. Res., 48, doi:10.1029/2012WR011871, in press, 2012a.
Franz, T. E., Zreda, M., Rosolem, R., and Ferre, T. P. A.: A universal calibration function for determination of soil moisture with cosmic-ray neutrons, Hydrol. Earth Syst. Sci. Discuss., 9, 10303–10322, doi:10.5194/hessd-9-10303-2012, 2012b.
Franz, T. E., Zreda, M., Rosolem, R., and Ferre, P. A.: Field validation of cosmic-ray soil moisture sensor using a distributed sensor network, Vadose Zone J., 11, doi:10.2136/vzj2012.0046, in press, 2012c.
Gosse, J. C. and Phillips, F. M.: Terrestrial in situ cosmogenic nuclides: theory and application, Quaternary Sci. Rev., 20, 1475–1560, 2001.
Koren, V., Schaake, J., Mitchell, K., Duan, Q.-Y., and Chen, F.: A parameterization of snowpack and frozen ground intended for NCEP weather and climate models, J. Geophys. Res., 104, 19569–19585, 1999.
McKay, M. D., Beckman, R. J., and Conover, W. J.: A comparison of three methods for selecting values of input variables in the analysis of output from a computer code, Technometrics, 21, 239–245, doi:10.2307/1268522, 1979.
Pelowitz, D. B.: MCNPX User's Manual, version 5, LA-CP-05-0369, Los Alamos National Laboratory, Los Alamos, 2005.
Rosolem, R., Gupta, H. V., Shuttleworth, W. J., de Gon ¸calves, L. G. G., and Zeng, X.: Towards a comprehensive approach to parameter estimation in land surface parameterization schemes, Hydrol. Process., doi:10.1002/hyp.9362, in press, 2012.
Rosolem, R., Shuttleworth, W. J., Zreda M., Franz, T. E., and Zeng, X.: The effect of atmospheric water vapor on the cosmic-ray soil moisture signal, J. Hydrometeorol., in press, 2012.
Shuttleworth, W. J., Zreda, M., Zeng, X., Zweck, C., and Ferre, P. A.: The COsmic-ray Soil Moisture Observing System (COSMOS): a Non-Invasive, Intermediate Scale Soil Moisture Measurement Network, Proceedings of the British Hydrological Society's Third International Symposium: "Role of Hydrology in Managing Consequences of a Changing Global Environment", Newcastle University, 19–23 July 2010, ISBN:1903741173, 2010.
Vrugt, J. A. and Robinson, B. A.: Improved evolutionary optimization from genetically adaptive multimethod search, P. Natl. Acad. Sci. USA, 104, 708–711, 2007.

HESSD
10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

Zreda, M., Desilets, D., Ferre, T. P. A., and Scott, R. L.: Measuring soil moisture content non-invasively at intermediate spatial scale using cosmic-ray neutrons, Geophys. Res. Lett., 35, L21402, doi:10.1029/2008GL035655, 2008.

Zreda, M., Zeng, X., Shuttleworth, J., Zweck, C., Ferre, T., Franz, T., Rosolem, R., Desilets, D., Desilets, S., and Womack, G.: Cosmic-ray neutrons, an innovative method for measuring area-average soil moisture, GEWEX News, 21, 6–10, 2011.

Zreda, M., Shuttleworth, W. J., Zeng, X., Zweck, C., Desilets, D., Franz, T., Rosolem, R., and Ferre, T. P. A.: COSMOS: The COsmic-ray Soil Moisture Observing System, Hydrol. Earth Syst. Sci. Discuss., 9, 4505–4551, doi:10.5194/hessd-9-4505-2012, 2012.

Table 1. Site-specific values of ρ_s ($g\,cm^{-3}$), $\theta_{lattice}$ ($m^3\,m^{-3}$) and F, and the parameters N, α ($cm^3\,g^{-1}$) and L_3 ($g\,cm^{-2}$) obtained by calibrating the COSMIC model against MCNPX at the 42 COSMOS sites shown in Fig. 3 with $L_1 = 162.0\,g\,cm^{-2}$, $L_2 = 129.1\,g\,cm^{-2}$, and $L_4 = 3.16\,g\,cm^{-2}$.

Site name	Latitude (° N)	Longitude (° W)	ρ_s ($g\,cm^{-3}$)	$\theta_{lattice}$ ($m^3\,m^{-3}$)	F ($\times 10^{14}$) (–)	N (–)	α ($cm^3\,g^{-1}$)	L_3 ($g\,cm^{-2}$)
ARM-1	36.61	−97.49	1.40	0.075	8.07	510.5	0.239	107.8
Austin Cary	29.74	−82.22	1.42	0.004	4.47	247.3	0.290	110.3
Bondville	40.01	−88.29	1.45	0.058	11.43	708.2	0.240	113.1
Brookings	44.35	−96.84	1.40	0.042	6.97	430.5	0.245	106.1
Chestnut Ridge NOAA	35.93	−84.33	1.41	0.032	9.28	546.0	0.267	108.5
Coastal Sage UCI	33.73	−117.70	1.16	0.051	12.30	745.1	0.272	80.1
Daniel Forest	41.87	−111.51	1.14	0.033	5.62	326.4	0.298	79.1
Desert Chaparral UCI	33.61	−116.45	1.58	0.020	9.79	575.7	0.259	130.1
Fort Peck	48.31	−105.10	1.28	0.049	7.10	429.5	0.270	93.6
Harvard Forest	42.54	−72.17	0.89	0.042	10.59	613.4	0.327	56.0
Hauser Farm North	34.58	−111.86	1.36	0.033	9.27	556.0	0.262	102.3
Hauser Farm South	34.58	−111.86	1.50	0.039	8.05	482.6	0.251	120.5
Howland	45.20	−68.74	1.23	0.059	11.07	669.0	0.254	88.2
Iowa Validation Site	41.98	−93.69	1.53	0.069	7.87	507.1	0.224	124.3
Island Dairy	20.00	−155.29	0.69	0.144	7.63	469.8	0.306	50.0
JERC	31.24	−84.46	1.38	0.011	5.47	297.7	0.302	104.4
Kendall	31.74	−109.94	1.23	0.064	14.14	864.4	0.266	88.5
KLEE	0.28	36.87	1.00	0.058	11.29	691.3	0.291	64.5
Manitou Forest Ground	39.10	−105.10	1.40	0.039	7.17	434.9	0.259	106.9
Metolius	44.45	−121.56	1.04	0.044	6.41	378.3	0.312	69.4
Morgan Monroe	39.32	−86.41	1.38	0.041	9.00	543.5	0.257	105.0
Mozark	38.74	−92.20	1.43	0.053	9.25	557.1	0.252	109.9
Mpala North	0.49	36.87	1.45	0.041	5.99	353.0	0.269	114.0
Neb Field 3	41.16	−96.47	1.42	0.051	10.65	635.5	0.257	109.9
P301	37.07	−119.19	1.06	0.042	5.26	312.6	0.299	70.8
Park Falls	45.95	−90.27	1.26	0.021	6.44	365.5	0.299	90.7
Pe-de-Gigante	−21.62	−47.63	1.32	0.022	4.91	278.7	0.290	98.0
Rancho No Tengo	31.74	−110.02	1.40	0.044	6.77	394.2	0.274	107.5
Reynolds Creek	43.12	−116.72	0.90	0.052	7.26	433.4	0.318	57.0
Rietholzbach	47.38	8.99	0.94	0.047	9.22	542.0	0.306	60.9
Rosemount	44.71	−93.09	1.45	0.042	7.05	424.2	0.254	113.6
San Pedro 2	31.56	−110.14	1.40	0.056	7.77	464.9	0.262	107.3
Santa Rita Creosote	31.91	−110.84	1.46	0.037	7.65	463.4	0.251	114.8
Savannah River	33.38	−81.57	1.41	0.008	4.71	260.4	0.292	108.3
Silver Sword	19.77	−155.42	0.78	0.075	8.38	509.1	0.332	50.0
SMAP-OK	36.06	−97.22	1.46	0.076	7.46	475.3	0.232	115.6
Soaproot	37.03	−119.26	1.02	0.041	5.92	346.0	0.310	66.9
Sterling	38.97	−77.49	1.32	0.084	8.45	513.4	0.264	96.5
Tonzi Ranch	38.43	−120.97	1.48	0.076	9.83	628.5	0.232	118.0
UMBS	45.56	−84.71	1.29	0.005	4.74	268.8	0.293	94.4
UVA	37.92	−78.27	1.14	0.035	5.38	320.3	0.289	79.0
Wind River	45.82	−121.95	0.88	0.058	6.66	394.5	0.318	55.5
Mean	–	–	–	0.047	8.07	475.4	0.276	94.0
Standard Deviation	–	–	–	0.025	4.47	142.6	0.028	22.4

HESSD
10, 1097–1125, 2013

Table 2. Criteria that characterize the comparison between the different time series illustrated in Fig. 9.

	R^2	Root mean squared error ($m^3\,m^{-3}$)	Bias ($m^3\,m^{-3}$)
Noah model without data assimilation versus TDT	0.72	0.12	+0.12
Noah model with data assimilation versus TDT	0.87	0.01	+0.01
Noah model without data assimilation versus COSMOS probe estimate	0.88	0.11	+0.11
Noah model with data assimilation versus COSMOS probe estimate	0.96	0.01	+0.01
TDT versus COSMOS probe estimate	0.82	0.01	−0.00

HESSD
10, 1097–1125, 2013

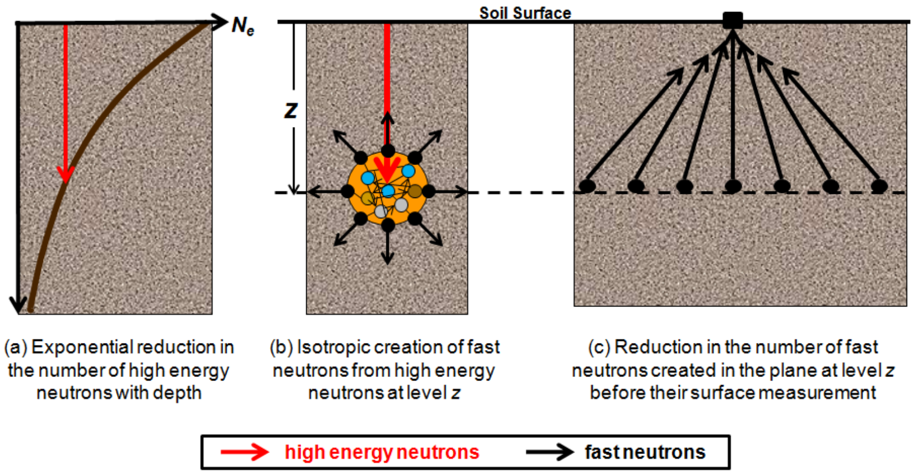

Fig. 1. The three physical processes represented in the COSMIC model that are assumed to control the above ground fast neutron count rate.

HESSD
10, 1097–1125, 2013

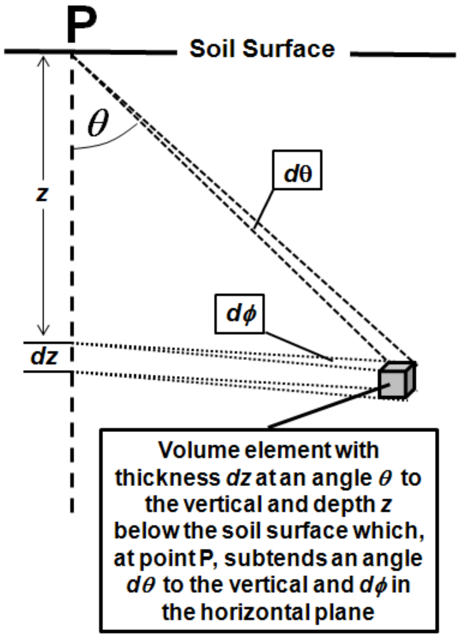

Fig. 2. The source volume element of fast neutrons created in the plane at depth z in the soil which may reach the measurement point P, but whose number is attenuated by an exponential factor with length constants L_3 and L_4 (in gm per unit area), these being respectively determined by the chemistry of the soil and by the total water content of the soil, including lattice water.

HESSD
10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

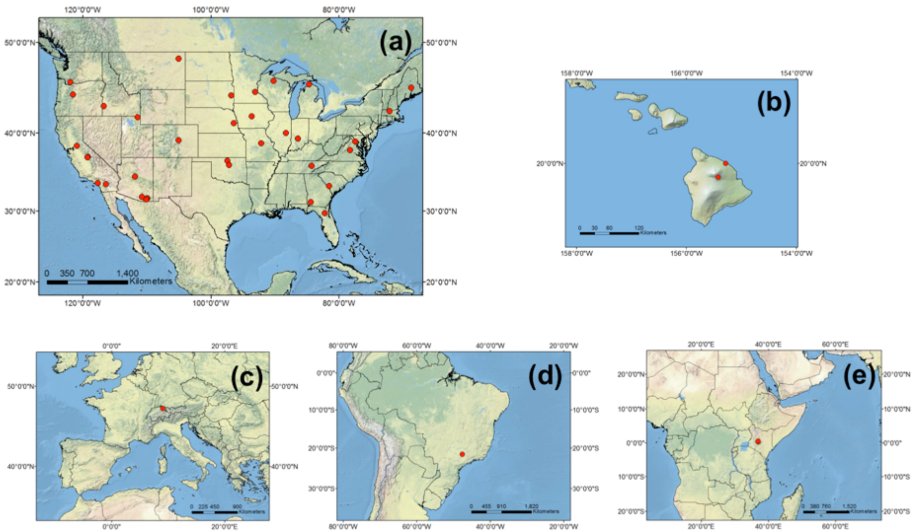

Fig. 3. The locations of the 42 sites in **(a)** the continental USA, **(b)** Hawaii, **(c)** Europe, **(d)** South America and **(e)** Africa for which optimization of the COSMIC model parameters given in Tables 1 were made (for site details, go to http://cosmos.hwr.arizona.edu/Probes/probemap.php and click on the site of interest).

HESSD

10, 1097–1125, 2013

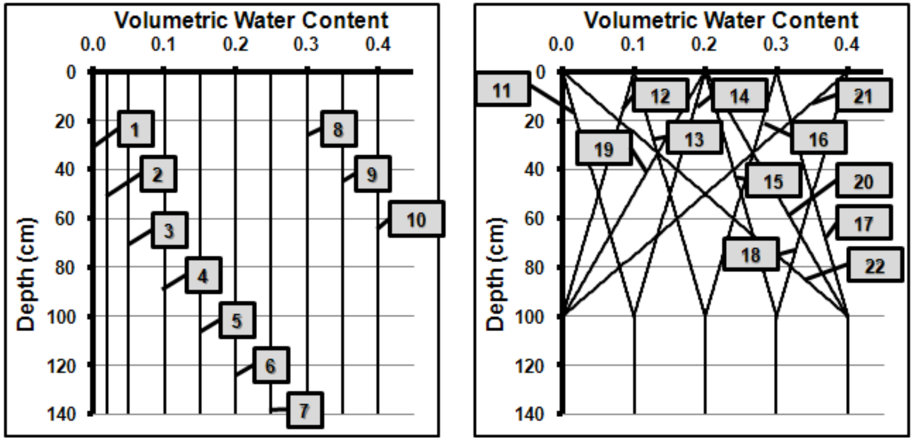

Fig. 4. The 22 prescribed profiles of soil water content (8 uniform and 12 with constant gradients) for which calculations of the above ground fast neutron count in the COSMOS detector are made using both MCNPX and COSMIC during parameter estimation.

HESSD
10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

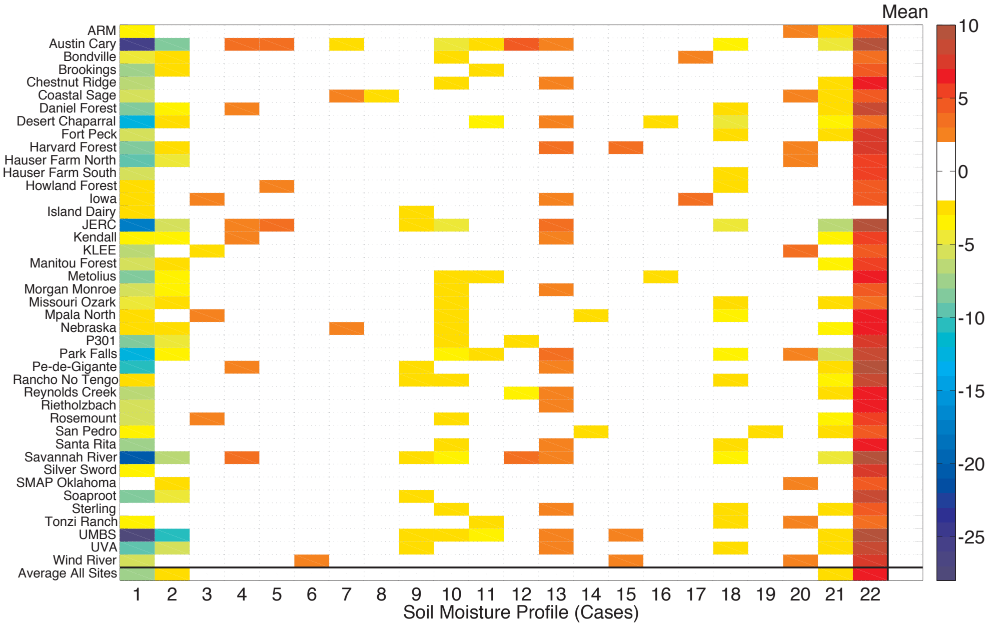

Fig. 5. Percentage difference illustrated by color (see key to the right) between the simulated neutron count given by COSMIC with optimized parameters and the neutron count given by MCNPX normalized by the MCNPX count for each of the sites shown in Fig. 3 and each of the hypothetical soil moisture profiles shown in Fig. 4. The last column (labeled Mean) shows the site-average difference, while the bottom row shows the average across all sites. For comparison, the typical observation error in a COSMOS probe is around 2 %.

HESSD

10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

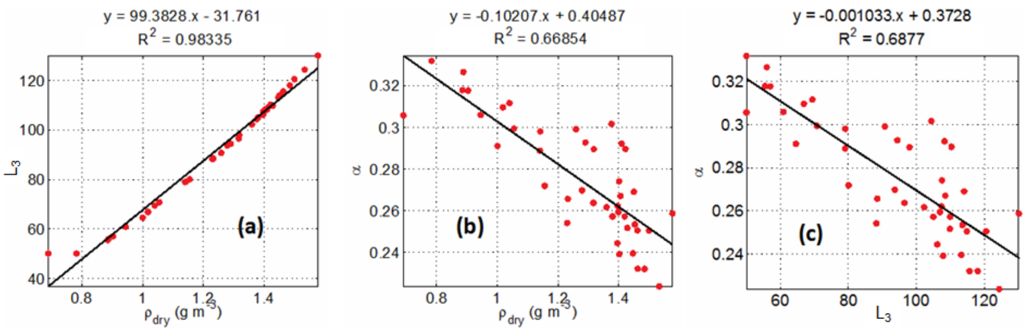

Fig. 6. Correlation of the site-specific optimized values of **(a)** L_3 and **(b)** α with the site-specific value of ρ_s, and **(c)** correlation between the site-specific optimized values of α and L_3.

HESSD
10, 1097–1125, 2013

The COsmic-ray Soil Moisture Interaction Code (COSMIC)

J. Shuttleworth et al.

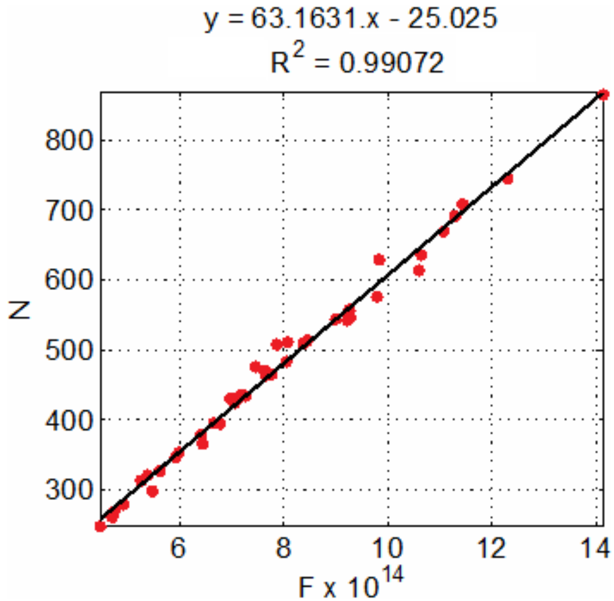

Fig. 7. Relationship between the COSMIC parameter N found by multi-parameter optimization and the factor F, this being the ratio between the number of counts observed during the COSMOS probe calibration at a specific site and the calculated neutron flux intensity given by MCNPX when run with the soil chemistry and water content (including lattice water) observed at each probe site during calibration.

HESSD
10, 1097–1125, 2013

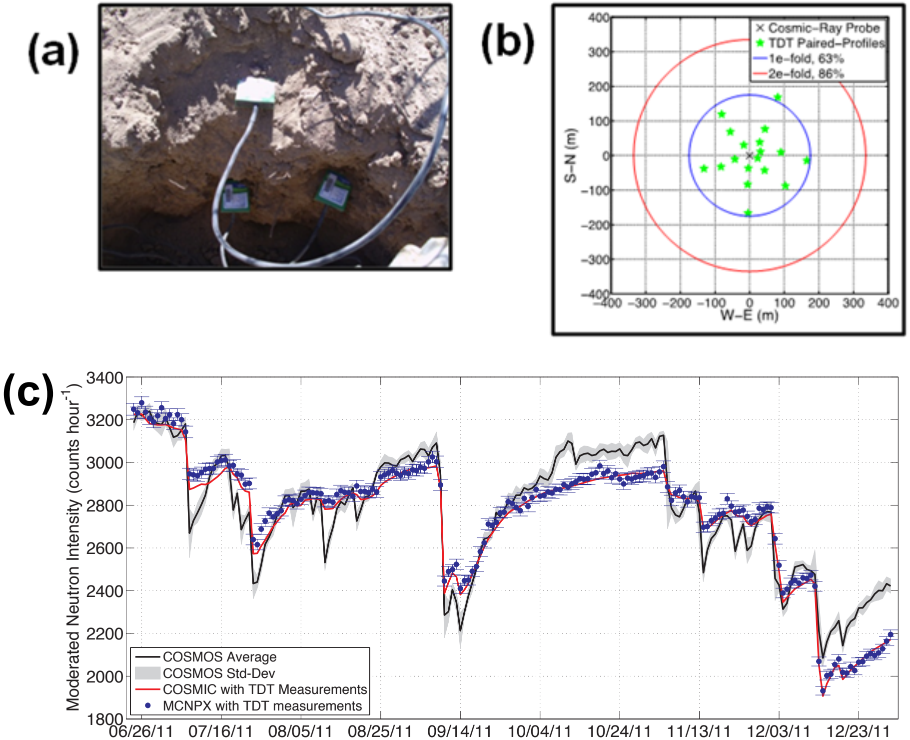

Fig. 8. At the Santa Rita Experimental Reserve field site, **(a)** the Time-Domain Transmission (TDT) probes installed at one of the soil profiles; **(b)** the locations at which the paired vertical profiles of TDT probes were installed within the footprint of the COSMOS probe (note the location of the TDT profiles are biased towards making measurements within the 1e-fold area sampled by the COSMOS probe); and **(c)** comparison between the fast neutron count observed by COSMOS probe (black) and that calculated using COSMIC (red) from the area-average soil moisture profile measured with TDT profiles.

HESSD
10, 1097–1125, 2013

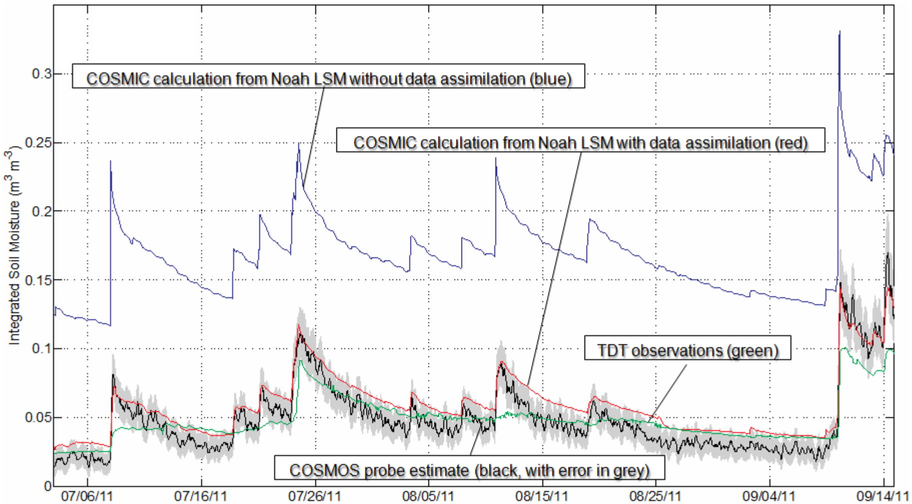

Fig. 9. Application of the COSMIC model to assimilate COSMOS probe counts into the Noah land surface model at the Santa Rita field site, showing time series of depth-average soil moisture (weighted by each level's contribution to the above ground fast neutron flux calculated by COSMIC) for the Noah model without data assimilation (blue), calculated by the Noah model with data assimilation (red), and the area average soil moisture measured by the TDT network (green). Also shown is the Level 3 soil moisture provided on the COSMOS website (black) together with an estimate of the error in this value (in grey) that allows both for neutron counting statistics and estimated error in the calibration function.

HESSD
10, 1097–1125, 2013