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Impact of gravels and organic matter on the thermal properties of grassland soils in southern France

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Abstract

Soil moisture is the main driver of temporal changes in values of the soil thermal conductivity. The latter is a key variable in land surface models (LSMs) used in hydrometeorology, for the simulation of the vertical profile of soil temperature in relation to soil moisture. Shortcomings in soil thermal conductivity models tend to limit the impact of improving the simulation of soil moisture in LSMs. Models of the thermal conductivity of soils are affected by uncertainties, especially in the representation of the impact of soil properties such as the volumetric fraction of quartz (q), soil organic matter, and gravels. As soil organic matter and gravels are often neglected in LSMs, the soil thermal conductivity models used in most LSMs represent the mineral fine earth, only. Moreover, there is no map of q and it is often assumed that this quantity is equal to the volumetric fraction of sand. In this study, q values are derived by reverse modelling from the continuous soil moisture and soil temperature sub-hourly observations of the Soil Moisture Observing System – Meteorological Automatic Network Integrated Application (SMOSMANIA) network at 21 grassland sites in southern France, from 2008 to 2015. The soil temperature observations are used to retrieve the soil thermal diffusivity (D_h) at a depth of 0.10 m in unfrozen conditions, solving the thermal diffusion equation. The soil moisture and D_h values are then used together with the measured soil properties to retrieve soil thermal conductivity (λ) values. For ten sites, the obtained λ value at saturation (λ_{sat}) cannot be retrieved or is lower than the value corresponding to a null value of q , probably in relation to a high density of grass roots at these sites or to the presence of stones. For the remaining eleven sites, q is negatively correlated with the volumetric fraction of solids other than sand. The impact of neglecting gravels and organic matter on λ_{sat} is assessed. It is shown that these factors have a major impact on λ_{sat} .

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1 Introduction

Soil thermal properties are characterized by two key variables: the soil volumetric heat capacity (C_h), and the soil thermal conductivity (λ), in $\text{J m}^{-3} \text{K}^{-1}$ and $\text{W m}^{-1} \text{K}^{-1}$, respectively. Provided the volumetric fractions of moisture, minerals and organic matter are known, C_h can be calculated easily. On the other hand, the estimation of λ relies on empirical models and is affected by uncertainties (Peters-Lidard et al., 1998 ; Tarawski et al., 2012). The construction and the verification of the λ models is not easy as λ is difficult to measure directly in situ and is often measured in the lab on perturbed soil samples (Abu-Hamdeh et al., 2000). Moreover, for given soil moisture conditions, λ depends to a large extent on the fraction of soil minerals presenting high thermal conductivities such as quartz, hematite, dolomite or pyrite (Côté and Conrad, 2005). At mid-latitudes, quartz is the main driver of λ . The fraction of quartz is generally unknown as it can only be measured using X-ray diffraction or X-ray fluorescence techniques, which are difficult to implement (Schönenberger et al., 2012).

Today, most of the Land Surface Models (LSMs) used in meteorology and hydrometeorology simulate λ following the approach proposed by Peters-Lidard et al. (1998). This approach consists of an updated version of the Johansen (1975) model, and assumes that the volumetric fraction of quartz (q) is equal to the volumetric fraction of sand (f_{sand}). This is a strong assumption, as some sandy soils (e.g. calcareous sands) may contain little quartz, and as quartz may be found in the silt and clay fractions of the soil minerals. Moreover, soil organic matter (SOM) and gravels are often neglected in LSMs, and the λ models used in most LSMs represent the mineral fine earth, only. Yang et al. (2005) and Chen et al. (2012) have shown the importance of accounting for SOM and gravels in λ models for organic top soil layers of grasslands of the Tibetan plateau.

In this study, an attempt is made to use routine automatic soil moisture and soil temperature sub-hourly measurements to retrieve instantaneous λ values at 21 weather stations of the Soil Moisture Observing System – Meteorological Automatic Network

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Integrated Application (SMOSMANIA) network (Calvet et al., 2007) in southern France, at a depth of 0.10 m. The response of λ to soil moisture is investigated and the feasibility of modelling the λ value at saturation (λ_{sat}) with or without using SOM and gravel fraction observations is assessed. The q values are retrieved by reverse modelling.

The field data and the method to retrieve λ values are presented in Sect. 2. The λ and q retrievals are presented in Sect. 3 together with a sensitivity analysis of λ_{sat} to SOM and gravel fractions. Finally, the results are discussed in Sect. 4, and the main conclusions are summarized in Sect. 5.

2 Data and methods

2.1 The SMOSMANIA data

The SMOSMANIA soil moisture network was developed by Calvet et al. (2007) in southern France in order to validate satellite-derived soil moisture products (Parrens et al., 2012), assess land surface models used in hydrological models (Draper et al., 2011) and in meteorological models (Albergel et al., 2010), and monitor the impact of climate change on water resources and droughts. The station network forms a transect between the Atlantic coast and the Mediterranean sea (Fig. 1). It consists of pre-existing automatic weather stations operated by Météo-France, upgraded with four soil moisture probes at four depths: 0.05, 0.10, 0.20, and 0.30 m. In general, the stations are located on former cultivated fields and consist of grasslands. Soil properties were measured at each stations using soil samples collected during the installation of the probes. The 21 stations cover a very large range of soil texture characteristics (Fig. 2). At the same time, Fig. 2 shows that soil texture does not vary much with depth (from 0.05 to 0.20 m) at a given station. Other properties such as the gravimetric fraction of the Soil Organic Matter (SOM) and of gravels were determined from the soil samples. In addition, the bulk dry density of the soil (ρ_d) was measured using unperturbed oven-dried soil samples collected using metal cylinders of known volume (about $7 \times 10^{-4} \text{ m}^3$).

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Twelve SMOSMANIA stations were activated in 2006 in southwestern France. In 2008, nine more stations were installed along the Mediterranean coast, and the whole network (21 stations) was gradually equipped with temperature sensors at the same depths as soil moisture probes. The soil moisture and soil temperature probes consisted of Thetaprobe ML2X and PT100 sensors, respectively.

The ThetaProbe sensors provide a voltage signal in units of V. In order to convert the voltage signal into volumetric soil moisture content ($\text{m}^3 \text{m}^{-3}$), site-specific calibration curves were developed using in situ gravimetric soil samples for all stations, and for all depths (Albergel et al., 2008). In this study, the calibration was revised in order to avoid spurious high soil moisture values during intense precipitation events. Logistics curves were used instead of exponential curves in the previous version of the data set.

The soil temperature observations are recorded with a resolution of 0.1°C .

The observations from the 48 soil moisture probes and from the 48 temperature probes are automatically recorded every 12 min. The data are available to the research community through the International Soil Moisture Network web site (<https://ismn.geotuwien.ac.at/>).

Figure 3 shows soil temperature time series at the Saint-Félix-de-Lauragais (SFL) station on 23 February 2015. The impact of recording temperature with a resolution of 0.1°C is clearly visible at all depths as this causes a levelling of the curves.

In this study, sub-hourly measurements of soil temperature and soil moisture at a depth of 0.10 m are used, together with soil temperature measurements at 0.05 and 0.20 m, from 1 January 2008 to 28 February 2015.

2.2 Soil characteristics

The porosity values at a depth of 0.10 m are listed in Table 1 together with gravimetric and volumetric fractions of soil particle-size ranges (sand, clay, silt, gravel) and SOM. The porosity, or soil volumetric moisture at saturation (θ_{sat}), is derived from the bulk dry

density ρ_d , together with soil texture and soil organic matter observations as:

$$\theta_{\text{sat}} = 1 - \rho_d \left[\frac{m_{\text{sand}} + m_{\text{clay}} + m_{\text{silt}} + m_{\text{gravel}}}{\rho_{\text{min}}} + \frac{m_{\text{SOM}}}{\rho_{\text{SOM}}} \right]$$

or

$$\theta_{\text{sat}} = 1 - f_{\text{sand}} - f_{\text{clay}} - f_{\text{silt}} - f_{\text{gravel}} - f_{\text{SOM}}, \quad (1)$$

5 where m_x (f_x) represents the gravimetric (volumetric) fraction of the soil component x . The f_x values are derived from the measured gravimetric fractions, multiplied by the ratio of ρ_d observations to ρ_x , the density of each soil component x . Values of $\rho_{\text{SOM}} = 1300 \text{ kg m}^{-3}$ and $\rho_{\text{min}} = 2660 \text{ kg m}^{-3}$ are used for soil organic matter, and soil minerals, respectively.

10 2.3 Retrieval of soil thermal diffusivity

The soil thermal diffusivity (D_h) is expressed in $\text{m}^2 \text{ s}^{-1}$ and is defined as:

$$D_h = \frac{\lambda}{C_h} \quad (2)$$

15 In this study, a simple numerical method is used to retrieve instantaneous values of D_h at a depth of 0.10 m using three soil temperature observations at 0.05, 0.10 and 0.20 m, performed every 12 min, by solving the Fourier thermal diffusion equation. The latter can be written as:

$$C_h \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right). \quad (3)$$

In this study, given that soil properties are relatively homogeneous on the vertical (Sect. 2.1), values of D_h can be derived from the Fourier one-dimensional law:

$$20 \frac{\partial T}{\partial t} = D_h \frac{\partial^2 T}{\partial z^2} \quad (4)$$

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2.6 Reverse modelling

The λ_{sat} values are retrieved through reverse modelling using the λ model described above (Eqs. 7–11). The λ model is used to produce simulations of λ at the same soil moisture conditions as those encountered for the λ values derived from observations in Sect. 2.4. For a given station, a set of 401 λ simulations is produced for λ_{sat} ranging from 0 to $4 \text{ W m}^{-1} \text{ K}^{-1}$, with a resolution of $0.01 \text{ W m}^{-1} \text{ K}^{-1}$. The λ_{sat} retrieval corresponds to the λ simulation presenting the lowest root mean square difference (RMSD) value with respect to the observations. Only λ observations for S_d values higher than 0.4 are used, as the λ_{sat} retrievals are very sensitive to uncertainties in λ observations obtained in dry conditions. Finally, the q value is derived from the retrieved λ_{sat} by solving Eq. (10), provided at least twenty λ observations can be used. When negative values of q are obtained, a null value of q is imposed

3 Results

3.1 λ_{sat} and q retrievals

Figure 4 shows retrieved and modelled λ values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for contrasting retrieved values of λ_{sat} (2.79, 1.45, and $0.70 \text{ W m}^{-1} \text{ K}^{-1}$) at the SBR, MNT, and PRD stations, respectively. All the obtained λ_{sat} and q retrievals are listed in Table 2, together with the λ RMSD values and the number of available λ observations. For six stations (CRD, PZN, MZN, VLV, MJN, and BRZ), the reverse modelling technique described in Sect. 2.6 cannot be implemented as not enough λ observations could be obtained for S_d values higher than 0.4. For the other 15 stations, λ_{sat} and q retrievals are obtained using 62 to 1939 λ observations. For the five stations (LHS, SVN, NBN, and PRD) presenting the lowest λ_{sat} retrievals, ranging between 0.52 and $1.11 \text{ W m}^{-1} \text{ K}^{-1}$, null values of q are obtained. The λ model (Eqs. 7–

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11) is fully operative, with non-null values of q , for eleven stations: SBR, URG, PRG, CDM, MNT, SFL, MTM, LZC, LGC, BRN, CBR.

3.2 A pedotransfer function for quartz

The q retrievals can be used to assess the possibility to estimate q using other soil characteristics, which can be easily measured.

For the 11 stations with $q > 0$, a good correlation is found between q retrievals and f_{sand} ($r^2 = 0.66$, F test p value = 0.0025, $\text{RMSD} = 0.09 \text{ m}^3 \text{ m}^{-3}$). However, a better result is found considering the sum of the fractions of the other soil particles, and the modelled q values can be derived from the following pedotransfer function:

$$q_{\text{MOD}} = 0.70 - 1.075 \times (f_{\text{clay}} + f_{\text{silt}} + f_{\text{gravel}} + f_{\text{SOM}})$$

$$\text{or } q_{\text{MOD}} = 0.70 - 1.075 \times (1 - \theta_{\text{sat}} - f_{\text{sand}}) \quad (12)$$

($r^2 = 0.78$, F test p value = 0.0003, $\text{RMSD} = 0.07 \text{ m}^3 \text{ m}^{-3}$). The values of q_{MOD} vs. q are shown in Fig. 5.

Modelled values of λ_{sat} (λ_{satMOD}) can be derived from q_{MOD} using Eq. (10) and the following r^2 , RMSD , and mean bias scores are obtained for λ_{satMOD} , with respect to the λ_{sat} retrievals: 0.87, $0.15 \text{ W m}^{-1} \text{ K}^{-1}$, and $-0.01 \text{ W m}^{-1} \text{ K}^{-1}$, respectively (Table 3).

Finally, we investigated the possibility of estimating θ_{sat} from the soil characteristics listed in Table 1 and of deriving a statistical model for θ_{sat} (θ_{satMOD}). We found the following statistical relationship between θ_{satMOD} , m_{clay} , m_{silt} , and m_{SOM} :

$$\theta_{\text{satMOD}} = 0.456 - 0.0735 \frac{m_{\text{clay}}}{m_{\text{silt}}} + 2.238 m_{\text{SOM}} \quad (13)$$

($r^2 = 0.48$, F test p value = 0.0027, $\text{RMSD} = 0.036 \text{ m}^3 \text{ m}^{-3}$).

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installation of the probes, it was observed that stones are present at the four stations. Stones are not evenly distributed in the soil, and it is not possible to investigate whether the soil area where the temperature probes were inserted contains stones as it must be left unperturbed.

5 4.3 Applicability of the new λ_{sat} model

The current global soil digital maps provide information about SOM, gravels and bulk density (Nachtergaele et al., 2012). Therefore, using Eq. (1) and Eqs. (6)–(12) at large scale is possible, and porosity can be derived from Eq. (1).

5 A key component of the λ_{sat} model proposed in this study is the pedotransfer function for quartz (Eq. 12). This equation should be evaluated for other regions. In particular, hematite has to be considered together with quartz for tropical soils. According to Eq. (12), q is close to 0.7 for sandy soils and in such conditions, one should ensure that $q \leq f_{\text{sand}}$.

15 While the pedotransfer function we get for θ_{sat} (Eq. 13) is valid for the specific sites considered in this study and is used to conduct the sensitivity study of Sect. 4.1, Eq. (13) cannot be used to predict porosity in other regions.

4.4 Prospects for using soil temperature profiles

A key limitation of the data used in this study is that soil temperature observations (T_i) are recorded with a resolution of $\Delta T_i = 0.1^\circ\text{C}$ only (see Sect. 2.1).

20 Since T_i is recorded with a resolution of

$$\Delta T_i = \left| \partial \left(T_i^n - T_i^{n-1} \right) \right| = \left| \partial \left(T_{i+1}^n - T_i^n \right) \right| = 0.1^\circ\text{C}, \quad (15)$$

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the retrieved D_h values are affected by uncertainties and the relative uncertainty of D_h can be estimated as:

$$\left| \frac{\partial D_{hi}}{D_{hi}} \right| = \Delta T_i \times \left\{ \frac{1}{|T_i^n - T_i^{n-1}|} + \frac{\Delta z_{i+1}^{-1} + \Delta z_i^{-1}}{|\gamma_{i+1}^n - \gamma_i^n| + |\gamma_{i+1}^{n-1} - \gamma_i^{n-1}|} \right\}. \quad (16)$$

Therefore, D_h retrievals are more accurate in conditions when soil temperature at $z_i = -0.10$ m changes rapidly and when differences in vertical gradients of soil temperature above and below z_i are more pronounced. In general, this occurs around noon (between 09:00 and 14:00 LST), and at dusk to a lesser extent, between 17:00 and 00:00 LST. In this study, we have imposed the following conditions for using the obtained D_h retrievals:

$$|T_i^n - T_i^{n-1}| > 0.8 \text{ }^\circ\text{C}, |\gamma_{i+1}^n - \gamma_i^n| > 30 \text{ Km}^{-1}, \text{ and } |\gamma_{i+1}^{n-1} - \gamma_i^{n-1}| > 30 \text{ Km}^{-1}. \quad (17)$$

According to Eq. (7), this ensures that

$$\left| \frac{\partial D_{hi}}{D_{hi}} \right| < 18\%. \quad (18)$$

It can be noticed that if T_i were recorded with a resolution of $0.03 \text{ }^\circ\text{C}$ (which corresponds to the typical uncertainty of PT100 probes), D_h could be retrieved with a precision of about 5% in the conditions of Eq. (17). Alternatively, Eq. (17) conditions could be relaxed in order to get more values of λ estimates for $S_d > 0.4$ (Sect. 2.6) and increase the number of usable stations. Therefore, one may recommend to revise the current practise of most observation networks consisting in recording soil temperature with a resolution of $0.1 \text{ }^\circ\text{C}$ only.

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5 Conclusions

An attempt was made to use routine soil temperature and soil moisture observations of a network of automatic weather stations to retrieve instantaneous values of the soil thermal conductivity at a depth of 0.10 m. The data from the SMOSMANIA network, in southern France, are used. First, the thermal diffusivity is derived from consecutive measurements of the soil temperature at a 48-minute interval, at three depths (0.05, 0.10, and 0.20 m). The thermal diffusion equation is solved using an implicit scheme. It is shown that, as the soil temperature records have a resolution of 0.1 °C, the thermal diffusivity can be obtained with a relative error of 18%. The λ values are then derived from the thermal diffusivity retrievals and from the volumetric heat capacity calculated using measured soil properties. The relationship between the λ estimates and the measured soil moisture at a depth of 0.10 m permits the retrieval of λ_{sat} for 15 stations. A classic λ model is then used to retrieve the quartz volumetric content by reverse modelling. For four stations, low values of λ_{sat} and null values of q are obtained, probably in relation to uncertainties in the gravel and stone fraction. For eleven stations, a pedotransfer function is proposed for quartz, for the considered region in France. A sensitivity study shows that gravels have a major impact on λ_{sat} and that omitting the SOM information tends to enhance this impact. This technique is easy to implement and is based on fully automatic in situ observations associated to a characterisation of soil properties in the lab. Therefore, this study could be extended to other regions and biomes. However, using temperature records with a resolution of 0.1 °C limits the applicability of the method. It is recommended to acquire temperature measurements with a better resolution. More precision in the λ estimates would then permit investigating other processes of heat transfer in the soil such as those related to water transport (Rutten, 2015).

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Table 2. λ_{sat} and q retrievals using the λ model (Eqs. 7–9 and Eq. 10, respectively) for degree of saturation values higher than 0.4, together with the minimized RMSD between the simulated and observed λ values, and the number of used λ observations (n). The four stations with $q = 0$ are in bold.

Station	Station full name	λ_{sat} ($\text{W m}^{-1} \text{K}^{-1}$)	q ($\text{m}^3 \text{m}^{-3}$)	RMSD ($\text{W m}^{-1} \text{K}^{-1}$)	n
SBR	SABRES	2.79	0.61	0.233	118
URG	URGONS	1.28	0.13	0.102	62
CRD	CREON-D'ARMAGNAC	–	–	–	0
PRG	PEYRUSSE-GRANDE	1.59	0.26	0.105	94
CDM	CONDOM	1.36	0.13	0.263	132
LHS	LAHAS	1.03	0.00	0.405	116
SVN	SAVENES	1.11	0.00	0.276	997
MNT	MONTAUT	1.45	0.38	0.103	207
SFL	SAINT-FELIX-DE-LAURAGAIS	1.40	0.14	0.183	1078
MTM	MOUTHOMET	1.45	0.18	0.137	1939
LZC	LEZIGNAN-CORBIERES	1.49	0.19	0.166	557
NBN	NARBONNE	0.52	0.00	0.101	100
PZN	PEZENAS	–	–	–	0
PRD	PRADES-LE-LEZ	0.70	0.00	0.165	490
LGC	LA-GRAND-COMBE	1.80	0.34	0.368	305
MZN	MAZAN-L'ABBAYE	–	–	–	0
VLV	VILLEVIEILLE	–	–	–	0
BRN	BARNAS	1.35	0.07	0.335	469
MJN	MEJANNES-LE-CLAP	–	–	–	0
BRZ	BERZEME	–	–	–	0
CBR	CABRIERES-D'AVIGNON	1.72	0.36	0.241	85

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Table 3. Ability of the Eqs. (10)–(13) empirical model to estimate λ_{sat} values at the 11 stations presenting non-null q values and impact of changes in the model, in order of decreasing r^2 score (from top to bottom). Results for all 15 stations (including null q values) are between brackets.

Model configuration	r^2	RMSD ($\text{W m}^{-1} \text{K}^{-1}$)	Mean bias ($\text{W m}^{-1} \text{K}^{-1}$)
Full model using θ_{sat} observations	0.87 (0.03)	0.15 (1.08)	−0.01 (+0.62)
Full model using θ_{satMOD} (Eqs. 13–14)	0.88 (0.01)	0.14 (1.02)	−0.03 (+0.62)
same with: $f_{\text{SOM}} = 0$	0.87 (0.00)	0.23 (1.18)	+0.12 (+0.78)
same with: $f_{\text{SOM}} = 0$ and $q = f_{\text{sand}}$	0.86 (0.02)	0.22 (1.06)	+0.00 (+0.64)
same with: $q = f_{\text{sand}}$	0.86 (0.12)	0.26 (0.82)	−0.22 (+0.37)
same with: $f_{\text{gravel}} = 0$ and $q = f_{\text{sand}}$	0.77 (0.17)	0.25 (0.81)	−0.15 (+0.39)
same with: $f_{\text{gravel}} = 0$	0.65 (0.07)	0.29 (1.06)	+0.15 (+0.73)
same with: $f_{\text{gravel}} = 0$, $f_{\text{SOM}} = 0$ and $q = f_{\text{sand}}$	0.61 (0.04)	0.42 (1.17)	+0.24 (+0.83)
same with: $f_{\text{gravel}} = 0$ and $f_{\text{SOM}} = 0$	0.51 (0.01)	0.56 (1.34)	+0.41 (+1.01)

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Table 4. Coefficient of determination and RMSD of the regression equation of q vs. diverse volumetric fractions of soil solids, for 11 SMOSMANIA stations. First line corresponds to the pedotransfer function for quartz proposed in this study (Eq. 12).

Predictor of q	r^2	RMSD ($\text{m}^3 \text{m}^{-3}$)
$f_{\text{clay}} + f_{\text{silt}} + f_{\text{gravel}} + f_{\text{SOM}}$	0.78	0.07
$f_{\text{clay}} + f_{\text{silt}} + f_{\text{gravel}}$	0.78	0.07
$f_{\text{silt}} + f_{\text{gravel}} + f_{\text{SOM}}$	0.67	0.09
f_{sand}	0.66	0.09
$f_{\text{clay}} + f_{\text{gravel}} + f_{\text{SOM}}$	0.38	0.12
$f_{\text{clay}} + f_{\text{silt}} + f_{\text{SOM}}$	0.12	0.14
$f_{\text{sand}} + f_{\text{gravel}}$	0.11	0.14

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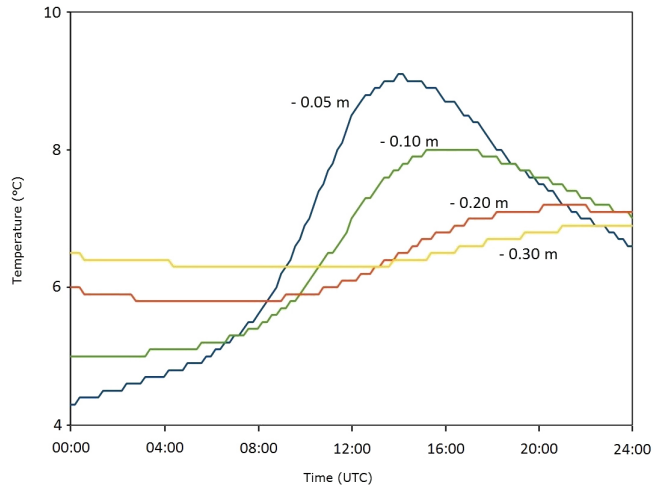


Figure 2. Soil characteristics of the 21 SMOSMANIA stations at a depth of 10 cm: mineral fine earth gravimetric fractions of clay, silt and sand. For a given station, the red mark covers the fraction values measured at 0.05, 0.10 and 0.20 m. Full station names are given in Table 2. The dashed blue lines correspond to the USDA textural soil classification.

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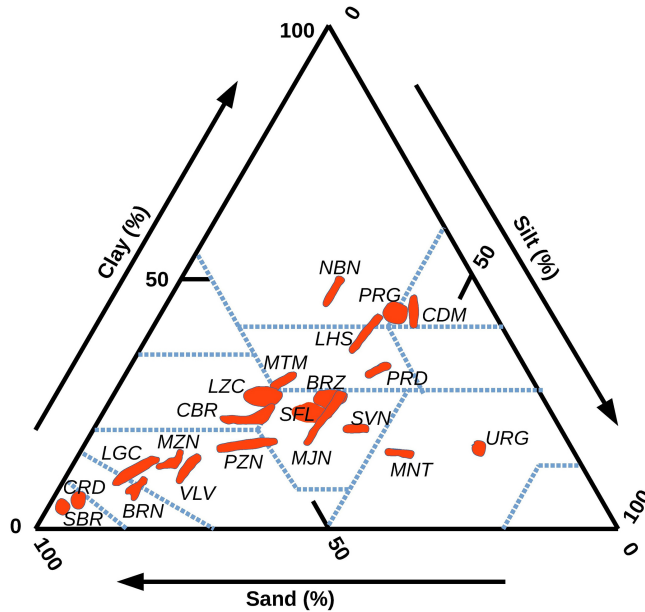


Figure 3. Soil temperature measured at the Saint-Félix-de-Lauragais (SFL) station on 23 February 2015, at depths of 0.05, 0.10, 0.20, and 0.30 m. Levelling is due to the low resolution of the temperature records (0.1 °C).

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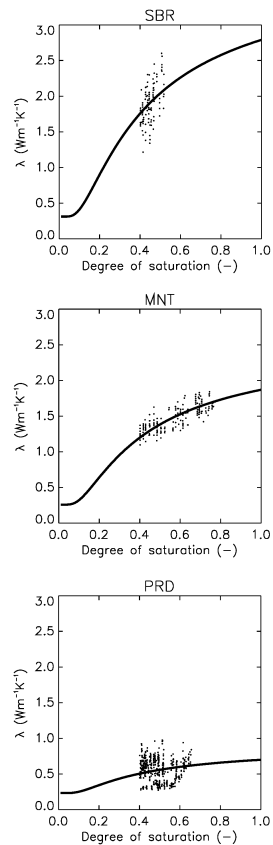


Figure 4. Retrieved λ values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for (from top to bottom) Sabres (SBR), Montaut (MNT), and Prades-le-Lez (PRD).

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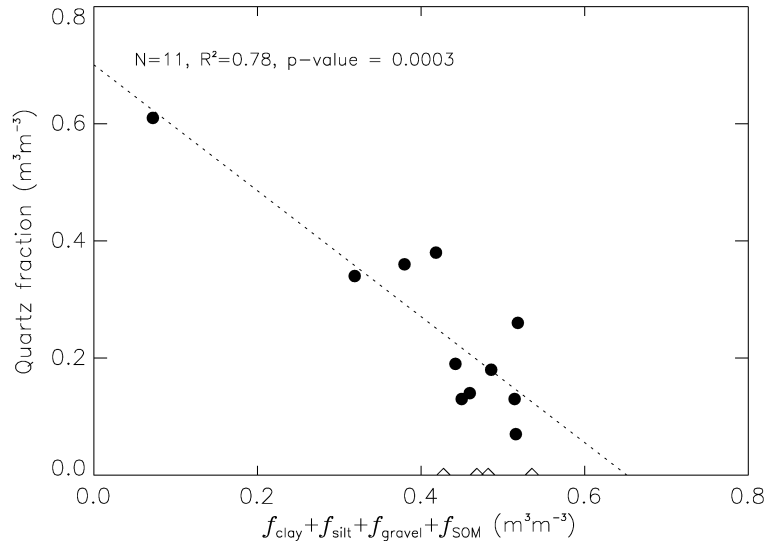


Figure 5. Non-null and null q retrievals (dark dots and opened diamonds, respectively) vs. the sum of clay, silt, gravel and SOM volumetric fractions (empirical Eq. 12).

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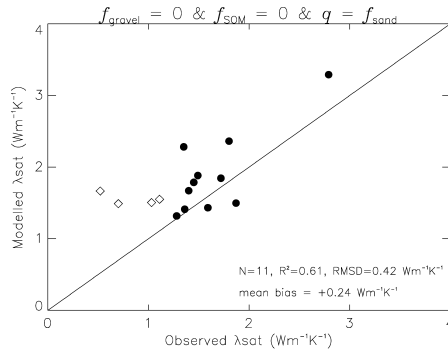
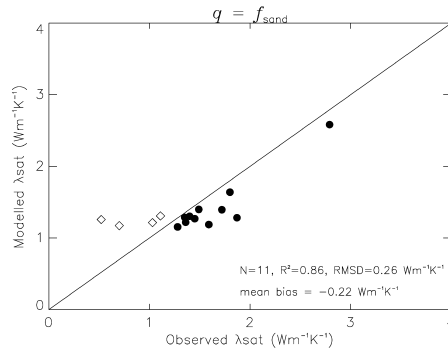
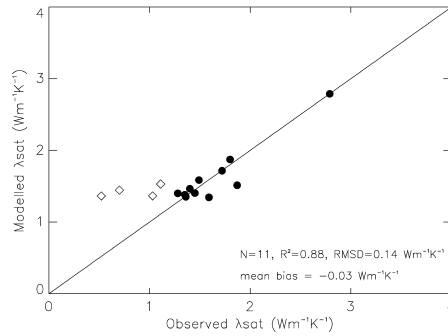


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Figure 6. λ_{satMOD} vs. λ_{sat} retrievals for non-null and null q retrievals (dark dots and opened diamonds, respectively): (top) full model using θ_{satMOD} (Eqs. 13–14), (middle) replacing Eq. (12) by $q = f_{\text{sand}}$, (bottom) replacing Eq. (12) by $q = f_{\text{sand}}$ and assuming $f_{\text{gravel}} = 0$ and $f_{\text{SOM}} = 0$ (Table 3).

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