1	Impact of quartz on the thermal properties of grassland soils in
2	southern France
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15	Abstract
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17	The information on quartz fraction in soils is usually unavailable but has a major effect on
18	the accuracy of soil thermal conductivity models and on their application in land surface
19	models. This paper investigates the influence of quartz fraction, soil organic matter (SOM)
20	and gravels on soil thermal conductivity. Field observations of soil temperature and water
21	content from 21 weather stations in southern France, along with the information on soil
22	texture and bulk density, are used to estimate soil thermal diffusivity and heat capacity, and
23	then thermal conductivity. The quartz fraction is inversely estimated using an empirical
24	thermal conductivity model. Several pedotransfer functions for estimating quartz content
25	from soil texture information are analysed. It is found that the soil volumetric fraction of
26	quartz $(f_q)$ is systematically better correlated to soil characteristics than the gravimetric
27	fraction of quartz. More than 60 % of the variance of $f_q$ can be explained using indicators
28	based on the sand fraction. It is shown that SOM and (or) gravels may have a marked
29	impact on thermal conductivity values depending on which predictor of $f_q$ is used. For the
30	grassland soils examined in this study, the ratio of sand to SOM fractions is the best
31	predictor of $f_q$ . An error propagation analysis and a comparison with independent data

from Lu et al. (2007) show that the gravimetric fraction of sand is a better predictor of  $f_q$ when a larger variety of soil types is considered.

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# 39 **1. Introduction**

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41 Soil moisture is the main driver of temporal changes in values of the soil thermal conductivity. 42 The latter is a key variable in land surface models (LSMs) used in hydrometeorology, for the 43 simulation of the vertical profile of soil temperature in relation to soil moisture. Shortcomings in 44 soil thermal conductivity models tend to limit the impact of improving the simulation of soil 45 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 46 47 quartz ( $f_q$ ), 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 48 49 earth, only. Today,  $f_q$  estimates are not given in global digital soil maps and it is often assumed 50 that this quantity is equal to the fraction of sand.

Soil thermal properties are characterized by two key variables: the soil volumetric heat capacity ( $C_h$ ), and the soil thermal conductivity ( $\lambda$ ), in Jm<sup>-3</sup>K<sup>-1</sup> and Wm<sup>-1</sup>K<sup>-1</sup>, 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  $\lambda$  relies on empirical models and is affected by uncertainties (Peters-Lidard et al., 1998 ; Tarnawski et al., 2012). The construction and the verification of the  $\lambda$  models is not easy as  $\lambda$  is often measured in the lab on perturbed soil samples (Abu-Hamdeh et al., 2000; Lu et al., 2007). Although recent advances in line-source

probe and heat pulse methods have made it easier to monitor soil thermal conductivity in the field 58 59 (Bristow et al., 1994; Zhang et al., 2014), such measurements are currently not made in 60 operational meteorological networks. Moreover, for given soil moisture conditions,  $\lambda$  depends to 61 a large extent on the fraction of soil minerals presenting high thermal conductivities such as 62 quartz, hematite, dolomite or pyrite (Côté and Conrad, 2005). At mid-latitudes, quartz is the main 63 driver of  $\lambda$ . The information on quartz fraction in a soil is usually unavailable as it can only be measured using X-ray diffraction or X-ray fluorescence techniques, which are difficult to 64 implement (Schönenberger et al., 2012). This has a major effect on the accuracy of thermal 65 66 conductivity models and their applications (Bristow, 1998).

67 Today, most of the Land Surface Models (LSMs) used in meteorology and hydrometeorology simulate  $\lambda$  following the approach proposed by Peters-Lidard et al. (1998). This approach 68 69 consists of an updated version of the Johansen (1975) model, and assumes that the gravimetric 70 fraction of quartz (Q) is equal to the gravimetric fraction of sand within mineral fine earth. This is 71 a strong assumption, as some sandy soils (e.g. calcareous sands) may contain little quartz, and as 72 quartz may be found in the silt and clay fractions of the soil minerals. Moreover, soil organic 73 matter (SOM) and gravels are often neglected in LSMs, and the  $\lambda$  models used in most LSMs represent the mineral fine earth, only. Yang et al. (2005) and Chen et al. (2012) have shown the 74 75 importance of accounting for SOM and gravels in  $\lambda$  models for organic top soil layers of 76 grasslands of the Tibetan plateau.

In this study, an attempt is made to use routine automatic soil temperature sub-hourly
measurements to retrieve instantaneous soil thermal diffusivity values at 21 weather stations of
the Soil Moisture Observing System – Meteorological Automatic Network Integrated Application
(SMOSMANIA) network (Calvet et al., 2007) in southern France, at a depth of 0.10 m. Using

81	information on soil moisture, soil texture, soil gravel content, soil organic matter, and bulk
82	density, $\lambda$ values are derived from soil thermal diffusivity and heat capacity. The response of $\lambda$ to
83	soil moisture is investigated and the feasibility of modelling the $\lambda$ value at saturation ( $\lambda_{sat}$ ) with or
84	without using SOM and gravel fraction observations is assessed using an empirical thermal
85	conductivity model based on Lu et al. (2007). The volumetric fraction of quartz, $f_q$ , is retrieved by
86	reverse modelling together with $Q$ . Pedotransfer functions are further proposed for estimating
87	quartz content from soil texture information.
88	The field data and the method to retrieve $\lambda$ values are presented in Sect. 2. The $\lambda$ and $f_q$ retrievals
89	are presented in Sect. 3 together with a sensitivity analysis of $\lambda_{sat}$ to SOM and gravel fractions.
90	Finally, the results are discussed in Sect. 4, and the main conclusions are summarized in Sect. 5.
91	Technical details are given in Supplements.
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	2. Data and methods
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93 94 95 96 97 98 99 100	2.1. The SMOSMANIA data The SMOSMANIA soil moisture network was developed by Calvet et al. (2007) in southern
<ul> <li>93</li> <li>94</li> <li>95</li> <li>96</li> <li>97</li> <li>98</li> <li>99</li> <li>100</li> <li>101</li> </ul>	<ul><li>2.1. The SMOSMANIA data</li><li>The SMOSMANIA soil moisture network was developed by Calvet et al. (2007) in southern</li><li>France in order to validate satellite-derived soil moisture products (Parrens et al., 2012), assess</li></ul>
<ul> <li>93</li> <li>94</li> <li>95</li> <li>96</li> <li>97</li> <li>98</li> <li>99</li> <li>100</li> <li>101</li> <li>102</li> </ul>	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

106 upgraded with four soil moisture probes at four depths: 0.05 m, 0.10 m, 0.20 m, and 0.30 m. In 107 general, the stations are located on former cultivated fields and consist of grasslands. Soil 108 properties were measured at each stations using soil samples collected during the installation of 109 the probes. The 21 stations cover a very large range of soil texture characteristics (see 110 Supplement 1). Other properties such as the gravimetric fraction of the Soil Organic Matter 111 (SOM) and of gravels were determined from the soil samples. In addition, the bulk dry density of the soil  $(\rho_d)$  was measured using unperturbed oven-dried soil samples collected using metal 112 cylinders of known volume (about  $7 \times 10^{-4}$  m<sup>3</sup>). 113

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 ( $m^3 m^{-3}$ ), 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 (see Supplement 1) instead of exponential curves in the previous version of the data set.

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

126 The observations from the 48 soil moisture probes and from the 48 temperature probes are 127 automatically recorded every 12 minutes. The data are available to the research community 128 through the International Soil Moisture Network web site (https://ismn.geo.tuwien.ac.at/). Figure 2 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

131 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 m and 0.20 m, from 1 January
2008 to 30 September 2015.

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136 2.2. Soil characteristics

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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 ( $\theta_{sat}$ ), is derived from the bulk dry density  $\rho_d$ , together with soil texture and soil organic matter observations as:

142 
$$\theta_{sat} = 1 - \rho_d \left[ \frac{m_{sand} + m_{clay} + m_{silt} + m_{gravel}}{\rho_{min}} + \frac{m_{SOM}}{\rho_{SOM}} \right]$$

143 or

144 
$$\theta_{sat} = 1 - f_{sand} - f_{clay} - f_{silt} - f_{gravel} - f_{SOM}$$
(1)

145 where  $m_x$  ( $f_x$ ) represents the gravimetric (volumetric) fraction of the soil component x. The  $f_x$ 146 values are derived from the measured gravimetric fractions, multiplied by the ratio of  $\rho_d$ 147 observations to  $\rho_x$ , the density of each soil component x. Values of  $\rho_{SOM} = 1300$  kg m<sup>-3</sup> and  $\rho_{min} =$ 148 2660 kg m<sup>-3</sup> are used for soil organic matter, and soil minerals, respectively.

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### 151 2.3. Retrieval of soil thermal diffusivity

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153 The soil thermal diffusivity  $(D_h)$  is expressed in m<sup>2</sup>s<sup>-1</sup> and is defined as:

$$154 D_h = \frac{\lambda}{C_h} (2)$$

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

158 
$$C_h \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( \lambda \frac{\partial T}{\partial z} \right)$$
 (3).

159 In this study, given that soil properties are relatively homogeneous on the vertical (Sect. 2.1), 160 values of  $D_{\rm h}$  can be derived from the Fourier one-dimensional law:

161 
$$\frac{\partial T}{\partial t} = D_h \frac{\partial^2 T}{\partial z^2}$$
(4).

However, large differences in soil bulk density, from the top soil layer to deeper soil layers were observed for some soils (see Supplement 1). In order to limit this effect as much as possible, we only used the soil temperature data presenting a relatively low vertical gradient close to the soil surface, where most differences with deeper layers are found. This data sorting procedure is described in Supplement 2.

Given that three soil temperatures  $T_i$  (*i* ranging from 1 to 3) are measured at depths  $z_1 = -0.05$  m,  $z_2 = -0.10$  m, and  $z_3 = -0.20$  m, the soil diffusivity  $D_{hi}$  at  $z_i = z_2 = -0.10$  m can be obtained by solving the one-dimensional heat equation, using a finite difference method based on the implicit Crank-Nicholson scheme. When three soil depths are considered,  $z_{i-1}$ ,  $z_i$ ,  $z_{i+1}$ , the change in soil 171 temperature  $T_i$  at depth  $z_i$ , from time  $t_{n-1}$  to time  $t_n$ , within the time interval  $\Delta t = t_n - t_{n-1}$  can be 172 written as:

173 
$$\frac{T_i^n - T_i^{n-1}}{\Delta t} = D_{hi} \left[ \frac{1}{2} \left( \frac{\gamma_{i+1}^n - \gamma_i^n}{\Delta z_m} \right) + \frac{1}{2} \left( \frac{\gamma_{i+1}^{n-1} - \gamma_i^{n-1}}{\Delta z_m} \right) \right] \text{ with }$$

174 
$$\gamma_i^n = \frac{T_i^n - T_{i-1}^n}{\Delta z_i}, \Delta z_m = \frac{\Delta z_i + \Delta z_{i+1}}{2}, \text{ and } \Delta z_i = z_i - z_{i-1}$$
 (5).

176 In this study,  $\Delta z_i = -0.05$  m,  $\Delta z_{i+1} = -0.10$  m, and a value of  $\Delta t = 2880$  s (48 minutes) is used.

177 It is important to ensure that  $D_h$  retrievals are related to diffusion processes only and not to the 178 transport of heat by water infiltration or evaporation (Parlange et al., 1998; Schelde et al., 1998). 179 Therefore, only situations for which changes in soil moisture at all depths do not exceed 0.001 180 m<sup>3</sup>m<sup>-3</sup> within the  $\Delta t$  time lag are considered.

181

## 182 2.4. From soil diffusivity to soil thermal conductivity

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185 The observed soil properties and volumetric soil moisture are used to calculate the soil 186 volumetric heat capacity  $C_h$  at a depth of 0.10 m, using the de Vries (1963) mixing model. The  $C_h$ 187 values, in units of Jm<sup>-3</sup>K<sup>-1</sup>, are calculated as:

188 
$$C_h = \theta C_{h \, water} + f_{\min} C_{h \min} + f_{SOM} C_{hSOM}$$
(6)

189 where  $\theta$  and  $f_{min}$  represent the volumetric soil moisture and the volumetric fraction of soil 190 minerals, respectively. Values of  $4.2 \times 10^6 \text{ Jm}^{-3} \text{K}^{-1}$ ,  $2.0 \times 10^6 \text{ Jm}^{-3} \text{K}^{-1}$ , and  $2.5 \times 10^6 \text{ Jm}^{-3} \text{K}^{-1}$ , are used 191 for  $C_{hwater}$ ,  $C_{hmin}$ ,  $C_{hSOM}$ , respectively.

192 The  $\lambda$  values at 0.10 m are then derived from the  $D_{\rm h}$  and  $C_{\rm h}$  estimates (Eq. (2)).

194 2.5. Soil thermal conductivity model

195

196 In dry conditions, soils present low thermal conductivity values ( $\lambda_{dry}$ ). Experimental evidence 197 show that  $\lambda_{dry}$  is negatively correlated with porosity. For example, Lu et al. (2007) give:

198 
$$\lambda_{dry} = 0.51 - 0.56 \times \theta_{sat}$$
 (in Wm<sup>-1</sup>K<sup>-1</sup>) (7)

199 When soil pores are gradually filled with water,  $\lambda$  tends to increase towards a maximum value at 200 saturation ( $\lambda_{sat}$ ). Between dry and saturation conditions,  $\lambda$  is expressed as:

$$\lambda = \lambda_{dry} + K_e \left( \lambda_{sat} - \lambda_{dry} \right)$$
(8)

where,  $K_e$  is the Kersten number. The latter is related to the volumetric soil moisture,  $\theta$ , i.e. to the degree of saturation ( $S_d$ ). In this study, the formula recommended by Lu et al. (2007) is used:

204 
$$K_e = \exp\{\alpha (1 - S_d^{(\alpha - 1.33)})\},\$$

205 with  $\alpha = 0.96$  for  $Mn_{\text{sand}} \ge 0.4$  kg kg<sup>-1</sup>,  $\alpha = 0.27$  for  $Mn_{\text{sand}} < 0.4$  kg kg<sup>-1</sup>, and

$$206 \quad S_d = \theta / \theta_{sat} \tag{9}$$

207  $Mn_{\text{sand}}$  represents the sand mass fraction of mineral fine earth (values are given in Supplement 1). 208 Following Peters-Lidard et al. (1998),  $\lambda_{other}$  is taken as 2.0 Wm<sup>-1</sup>K<sup>-1</sup> for soils with  $Mn_{\text{sand}} > 0.2$ 209 kg kg<sup>-1</sup>, and 3.0 Wm<sup>-1</sup>K<sup>-1</sup> otherwise. In this study  $Mn_{\text{sand}} > 0.2$  kg kg<sup>-1</sup> for all soils, except for 210 URG, PRG, and CDM.

211 The geometric mean equation for  $\lambda_{sat}$  proposed by Johansen (1975) for the mineral components 212 of the soil can be generalized to include the SOM thermal conductivity (Chen et al., 2012) as:

$$\ln(\lambda_{sat}) = f_q \ln(\lambda_q) + f_{other} \ln(\lambda_{other}) + \theta_{sat} \ln(\lambda_{water}) + f_{SOM} \ln(\lambda_{SOM})$$

where  $f_q$  is the volumetric fraction of quartz, and  $\lambda_q = 7.7 \text{ Wm}^{-1}\text{K}^{-1}$ ,  $\lambda_{other} = 2.0 \text{ Wm}^{-1}\text{K}^{-1}$ ,  $\lambda_{water} = 0.594 \text{ Wm}^{-1}\text{K}^{-1}$ ,  $\lambda_{SOM} = 0.25 \text{ Wm}^{-1}\text{K}^{-1}$  are the thermal conductivities of quartz, soil minerals other than quartz, water and SOM, respectively. The volumetric fraction of soil minerals other than quartz is defined as:

220 
$$f_{other} = 1 - f_q - \theta_{sat} - f_{SOM}$$
221 with  $f_q = Q \times (1 - \theta_{sat})$ 
222 (11)

223 2.6. Reverse modelling224

225 The  $\lambda_{sat}$  values are retrieved through reverse modelling using the  $\lambda$  model described above (Eqs. 226 (7)-(11)). The  $\lambda$  model is used to produce simulations of  $\lambda$  at the same soil moisture conditions as those encountered for the  $\lambda$  values derived from observations in Sect. 2.4. For a given station, a 227 set of 401 simulations is produced for  $\lambda_{sat}$  ranging from 0 Wm<sup>-1</sup>K<sup>-1</sup> to 4 Wm<sup>-1</sup>K<sup>-1</sup>, with a 228 resolution of 0.01  $\text{Wm}^{-1}\text{K}^{-1}$ . The  $\lambda_{\text{sat}}$  retrieval corresponds to the  $\lambda$  simulation presenting the 229 230 lowest root mean square difference (RMSD) value with respect to the  $\lambda$  observations. Only  $\lambda$ observations for  $S_d$  values higher than 0.4 are used because in dry conditions: (1) conduction is 231 232 not the only mechanism for heat exchange in soils, as the convective water vapour flux may 233 become significant (Schelde et al., 1998, Parlange et al. 1998), (2) the  $K_e$  functions found in the 234 literature display more variability, (3) the  $\lambda_{sat}$  retrievals are more sensitive to uncertainties in  $\lambda$ 235 observations. The threshold value of  $S_d = 0.4$  results from a compromise between the need of

(10)

236	limiting the influence of convection, of the shape of the $K_e$ function on the retrieved values of
237	$\lambda_{\rm sat}$ , and of using as many observations as possible in the retrieval process. Moreover, the data
238	filtering technique to limit the impact of soil heterogeneities, described in Supplement 2, is used
239	to select valid $\lambda$ observations.
240	Finally, the $f_q$ value is derived from the retrieved $\lambda_{sat}$ solving Eq. (10).
241	
242 243	2.7. Scores
244	Pedotransfer functions for quartz and $\lambda_{sat}$ are evaluated using the following scores:
245	• the Pearson correlation coefficient (r), and the squared correlation coefficient ( $r^2$ ) is used
246	to assess the fraction of explained variance,
247	• the RMSD,
248	• the Mean Absolute Error (MAE), i.e. the mean of absolute differences,
249	• the mean bias, i.e. the mean of differences.
250	In order to test the predictive and generalization power of the pedotransfer regression equations, a
251	simple bootstrapping resampling technique is used. It consists in calculating a new estimate of $f_q$
252	for each soil using the pedotransfer function obtained without using this specific soil. Gathering
253	these new $f_q$ estimates, one can calculate new scores with respect to the retrieved $f_q$ values. Also,
254	this method provides a range of possible values of the coefficients of the pedotransfer function
255	and permits assessing the influence of a given $f_q$ retrieval on the final result.
256	

256 **3. Results** 

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259 3.1.  $\lambda_{sat}$  and  $f_q$  retrievals

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Retrievals of  $\lambda_{sat}$  and  $f_q$  could be obtained for 14 soils. Figure 3 shows retrieved and modelled  $\lambda$ values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for contrasting retrieved values of  $\lambda_{sat}$ , from high to low  $\lambda_{sat}$  values (2.80, 1.96, 1.52, and 1.26 Wm<sup>-1</sup>K<sup>-1</sup>) at the SBR, MNT, MTM, and PRD stations, respectively.

All the obtained  $\lambda_{sat}$  and  $f_q$  retrievals are listed in Table 2, together with the  $\lambda$  RMSD values and 266 267 the number of selected  $\lambda$  observations. For three soils (CRD, MZN, and VLV), the reverse 268 modelling technique described in Sect. 2.6 could not be applied as not enough  $\lambda$  observations 269 could be obtained for S<sub>d</sub> values higher than 0.4. For four soils (NBN, PZN, BRZ, and MJN), all 270 the  $\lambda$  retrievals were filtered out as the obtained values were influenced by heterogeneities in soil 271 density (see Supplement 2). For the other 14 soils,  $\lambda_{sat}$  and  $f_q$  retrievals were obtained using a 272 subset of 20  $\lambda$  retrievals per soil, at most, corresponding to the soil temperature data presenting 273 the lowest vertical gradient close to the soil surface (Supplement 2).

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276

275 3.2 Pedotransfer functions for quartz

The  $f_q$  retrievals can be used to assess the possibility to estimate  $f_q$  using other soil characteristics, which can be easily measured. Another issue is whether volumetric or gravimetric fraction of quartz should be used. Figure 4 presents the fraction of variance  $(r^2)$  of Q and  $f_q$  explained by various indicators. A key result is that  $f_q$  is systematically better correlated to soil characteristics than Q. More than 60 % of the variance of  $f_q$  can be explained using indicators based on the sand fraction (either  $f_{\text{sand}}$  or  $m_{\text{sand}}$ ). The use of other soil mineral fractions does not give good correlations, even when they are associated to the sand fraction as shown by Fig. 4. For example, the  $f_{\text{gravel}}$  and  $f_{\text{gravel}}+f_{\text{sand}}$  indicators present low  $r^2$  values of 0.04 and 0.24, respectively.

The  $f_q$  values cannot be derived directly from the indicators as illustrated by Fig. 5: assuming  $f_q = f_{sand}$  tends to markedly underestimate  $\lambda_{sat}$ . Therefore, more elaborate pedotransfer equations are needed. They can be derived from the best indicators, using them as predictors of  $f_q$ . The modelled  $f_q$  is written as:

$$289 \quad f_{aMOD} = a_0 + a_1 \times P$$

290 and 
$$f_{qMOD} \le 1 - \theta_{sat} - f_{SOM}$$
 (12)

291 where *P* represents the predictor of  $f_q$ .

The  $a_0$  and  $a_1$  coefficients are given in Table 3 for four pedotransfer functions based on the best predictors of  $f_q$ . The pedotranfer functions are illustrated in Fig. 6. The scores are displayed in Table 4. The bootstrapping indicates that the SBR sandy soil has the largest individual impact on the obtained regression coefficients. This is why the scores without SBR are also presented in Table 4.

For the  $m_{\text{sand}}$  predictor, a  $r^2$  value of 0.56 is obtained without SBR, against a value of 0.67 when all the 14 soils are considered. An alternative to this  $m_{\text{sand}}$  pedotransfer function consists in considering only  $m_{\text{sand}}$  values smaller than 0.6 kg kg<sup>-1</sup> in the regression, thus excluding the SBR soil. The corresponding predictor is called  $m_{\text{sand}}^*$ . In this configuration, the sensitivity of  $f_q$  to  $m_{\text{sand}}$  is much increased (with  $a_1 = 0.944$ , against  $a_1 = 0.572$  with SBR). For SBR,  $f_q$  is overestimated by the  $m_{\text{sand}}^*$  equation but this is corrected by the  $f_{qMOD}$  limitation of Eq. (12), and in the end a better  $r^2$  score is obtained when the 14 soils are considered ( $r^2 = 0.74$ ).

Values of  $r^2$  larger than 0.7 are obtained for two predictors of  $f_q$ :  $m_{\text{sand}}/m_{\text{SOM}}$  and  $m_{\text{sand}}^*$ . A value 304 of  $r^2 = 0.65$  is obtained for  $1 - \theta_{sat} - f_{sand}$  (the fraction of soil solids other than sand). The 305  $m_{\rm sand}/m_{\rm SOM}$  predictor presents the best  $r^2$  and RMSD scores in all the configurations (regression, 306 307 bootstrap, and regression without SBR). Another characteristic of the  $m_{\text{sand}}/m_{\text{SOM}}$  pedotransfer 308 function is that the confidence interval for the  $a_0$  and  $a_1$  coefficients derived from bootstrapping is 309 narrower than for the other pedotransfer functions (Table 3), indicating a more robust relationship of  $f_q$  with  $m_{\text{sand}}/m_{\text{SOM}}$  than with other predictors. Modelled values of  $\lambda_{\text{sat}}$  ( $\lambda_{\text{satMOD}}$ ) can be derived 310 from  $f_{qMOD}$  using Eq. (10) together with  $\theta_{sat}$  observations. The  $\lambda_{satMOD} r^2$ , RMSD, and mean bias 311 scores are given in Table 5. Again, the best scores are obtained using the  $m_{\text{sand}}/m_{\text{SOM}}$  predictor of 312  $f_q$ , with  $r^2$ , RMSD, and mean bias values of 0.86, 0.14 Wm<sup>-1</sup>K<sup>-1</sup>, and +0.01 Wm<sup>-1</sup>K<sup>-1</sup>, respectively 313 314 (Fig. 7).

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

318 
$$\theta_{satMOD} = 0.456 - 0.0735 \frac{m_{clay}}{m_{silt}} + 2.238 m_{SOM}$$
 (13)

319 
$$(r^2 = 0.48, \text{ F-test } p \text{-value} = 0.0027, \text{ RMSD} = 0.036 \text{ m}^3 \text{m}^{-3}).$$

320 Volumetric fractions of soil components need to be consistent with  $\theta_{\text{satMOD}}$  and can be calculated 321 using the modelled bulk density values derived from  $\theta_{\text{satMOD}}$  using Eq. (1).

Equations (10) to (13) constitute an empirical end-to-end model of  $\lambda_{sat}$ . Table 5 shows that using  $\theta_{satMOD}$  (Eqs. (13) ) instead of the  $\theta_{sat}$  observations has little impact on the  $\lambda_{satMOD}$  scores.

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327 3.3. Impact of gravels and SOM on  $\lambda_{sat}$ 

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329 Gravels and SOM are often neglected in soil thermal conductivity models used in LSMs. The 330 Eqs. (10)-(13) empirical model obtained in Sect. 3.2 permits the assessment of the impact of  $f_{\text{gravel}}$ 331 and  $f_{\text{SOM}}$  on  $\lambda_{\text{sat}}$ . Table 5 shows the impact on  $\lambda_{\text{sat}MOD}$  scores of imposing a null value of  $f_{\text{gravel}}$  and 332 a small value of  $f_{\text{SOM}}$  to all the soils. The combination of these assumptions is evaluated, also.

Imposing  $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$  (the smallest  $f_{\text{SOM}}$  value, observed for CBR) has a limited impact on the scores, except for the  $m_{\text{sand}}/m_{\text{SOM}}$  pedotransfer function. In this case,  $\lambda_{\text{sat}}$  is overestimated by +0.20 Wm<sup>-1</sup>K<sup>-1</sup>, and  $r^2$  drops to 0.57.

Neglecting gravels ( $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$ ) also has a limited impact but triggers the underestimation (overestimation) of  $\lambda_{\text{sat}}$  for the  $m_{\text{sand}}/m_{\text{SOM}}$  ( $m_{\text{sand}}^*$ ) pedotransfer function, by -0.12 Wm<sup>-1</sup>K<sup>-1</sup> (+0.11 Wm<sup>-1</sup>K<sup>-1</sup>).

339 On the other hand, it appears that combining these assumptions has a marked impact on all the pedotransfer functions. Neglecting gravels and imposing  $f_{SOM} = 0.013 \text{ m}^3 \text{m}^{-3}$  has a major impact 340 on  $\lambda_{sat}$ : the modelled  $\lambda_{sat}$  is overestimated by all the pedotransfer functions (with a mean bias 341 ranging from +0.16  $\text{Wm}^{-1}\text{K}^{-1}$  to +0.24  $\text{Wm}^{-1}\text{K}^{-1}$ ) and  $r^2$  is markedly smaller, especially for the 342  $m_{\rm sand}$  and  $m_{\rm sand}^*$  pedotransfer functions. These results are illustrated in Fig. 8 in the case of the 343  $m_{\rm sand}^*$  pedotransfer function. Figure 8 also shows that using the  $\theta_{\rm sat}$  observations instead of 344 345  $\theta_{\text{satMOD}}$  (Eq. (13)) has little impact on  $\lambda_{\text{satMOD}}$  (Sect. 3.2) but tends to enhance the impact of neglecting gravels. A similar result is found with the  $m_{\text{sand}}$  pedotransfer function (not shown). 346

# 349 **4. Discussion**

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## 351 4.1. Sources of uncertainties in heat capacity estimates

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In this study, the de Vries (1963) mixing model is applied to estimate soil volumetric heat capacity, and a fixed value of  $2.0 \times 10^6$  Jm<sup>-3</sup>K<sup>-1</sup> is used for soil minerals (Eq. (6)). Soil-specific values for  $C_{\text{hmin}}$  may be more appropriate than using a constant standard value. For example, Tarara and Ham (1997) used a value of  $1.92 \times 10^6$  Jm<sup>-3</sup>K<sup>-1</sup>. However, we did not measure this quantity and we were not able to find such values in the literature.

We investigated the sensitivity of our results to these uncertainties, considering the following minimum and maximum  $C_{\text{hmin}}$  values:  $C_{\text{hmin}} = 1.92 \times 10^6 \text{ Jm}^{-3} \text{ K}^{-1}$  and  $C_{\text{hmin}} = 2.08 \times 10^6 \text{ Jm}^{-3}$  $K^{-1}$ . The impact of changes in  $C_{\text{hmin}}$  on the retrieved values of  $\lambda_{\text{sat}}$  and  $f_q$  is presented in Fig. 9. On average, a change of + (-)  $0.08 \times 10^6 \text{ Jm}^{-3} \text{ K}^{-1}$  in  $C_{\text{hmin}}$  triggers a change in  $\lambda_{\text{sat}}$  and  $f_q$  of + 1.7 % (- 1.8 %) and + 4.8 % (- 7.0 %), respectively.

The impact of changes in  $C_{\text{hmin}}$  on the regression coefficients of the pedotransfer functions is presented in Table 3 (last column). The impact is very small, except for the  $a_1$  coefficient of the  $m_{\text{sand}}^*$  pedotransfer function. However, even in this case, the impact of  $C_{\text{hmin}}$  on the  $a_1$  coefficient is much lower than the confidence interval given by the bootstrapping, indicating that the relatively small number of soils considered in this study (as in other studies, e.g. Lu et al. (2007)) is a larger source of uncertainty. Moreover, uncertainties in the  $f_{clay}$ ,  $f_{silt}$ ,  $f_{gravel}$ , or  $f_{SOM}$  fractions may be caused by (1) the natural heterogeneity of soil properties, (2) the living root biomass, (3) stones that may not be accounted for in the gravel fraction.

In particular, during the installation of the probes, it was observed that stones are present at some 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.

The grasslands considered in this study are not intensively managed. They consist of set-aside fields cut once or twice a year. Calvet et al. (1999) gave an estimate of 0.160 kg m<sup>-2</sup> for the root dry matter content of such soils for a site in southwestern France, with most roots contained in the 0.25m top soil layer. This represents a gravimetric fraction of organic matter smaller than 0.0005 kg kg<sup>-1</sup>, i.e. less than 4% of the lowest  $m_{SOM}$  values observed in this study (0.013 kg kg<sup>-1</sup>) or less than 5% of  $f_{SOM}$  values. We checked that increasing  $f_{SOM}$  values by 5% has negligible impact on heat capacity and on the  $\lambda$  retrievals.

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4.3. Applicability of the new 
$$\lambda_{sat}$$
 model to other soil types

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The  $\lambda_{sat}$  values found in this study are consistent with values reported by other authors. In this study,  $\lambda_{sat}$  values ranging between 1.26 Wm<sup>-1</sup>K<sup>-1</sup> and 2.80 Wm<sup>-1</sup>K<sup>-1</sup> are found (Table 2). Tarnawski et al. (2011) gave  $\lambda_{sat}$  values ranging between 2.5 Wm<sup>-1</sup>K<sup>-1</sup> and 3.5 Wm<sup>-1</sup>K<sup>-1</sup> for standard sands. Lu et al. (2007) gave  $\lambda_{sat}$  values ranging between 1.33 Wm<sup>-1</sup>K<sup>-1</sup> and 2.2 Wm<sup>-1</sup>K<sup>-1</sup>.

393 A key component of the  $\lambda_{sat}$  model is the pedotransfer function for quartz (Eq. (12)). The  $f_q$ 394 pedotranfer functions proposed in this study are based on basic soil characteristics. The current 395 global soil digital maps provide information about SOM, gravels and bulk density (Nachtergaele 396 et al., 2012). Therefore, using Eq. (1) and Eqs. (6)-(12) at large scale is possible, and porosity can 397 be derived from Eq. (1). On the other hand, the suggested  $f_q$  pedotranfer functions are obtained 398 for temperate grassland soils containing a rather large amount of organic matter, and are valid for 399  $m_{\rm sand}/m_{\rm SOM}$  ratio values lower than 40 (Table 2). These equations should be evaluated for other 400 regions. In particular, hematite has to be considered together with quartz for tropical soils. 401 Moreover, while the pedotransfer function we get for  $\theta_{sat}$  (Eq. (13)) is valid for the specific sites 402 considered in this study and is used to conduct the sensitivity study of Sect. 3.3, Eq. (13) cannot 403 be used to predict porosity in other regions.

404 In order to assess the applicability of the pedotransfer function for quartz obtained in this study, 405 we used the independent data from Lu et al. (2007) and Tarnawski et al. (2009), for ten Chinese 406 soils (see Supplement 3 and Table S3.1). These soils consist of reassembled sieved soil samples 407 and contain no gravel, while our data concern undisturbed soils. Moreover, most of these soils 408 contain very little organic matter and the  $m_{\rm sand}/m_{\rm SOM}$  ratio can be much larger that the  $m_{\rm sand}/m_{\rm SOM}$ 409 values measured at our grassland sites. For the 14 French soils used to determine pedotransfer 410 functions for quartz, the  $m_{\text{sand}}/m_{\text{SOM}}$  ratio ranges from 3.7 to 37.2 (Table 2). Only three soils of Lu 411 et al. (2007) present such low values of  $m_{\text{sand}}/m_{\text{SOM}}$ . The other seven soils of Lu et al. (2007) 412 present  $m_{\text{sand}}/m_{\text{SOM}}$  values ranging from 48 to 1328 (see Table S3.1).

413 We used  $\lambda_{sat}$  experimental values derived from Table 3 in Tarnawski et al. (2009) to calculate Q414 and  $f_q$  for the ten Lu et al. (2007) soils. Figure 10 shows the statistical relationship between these 415 quantities and  $m_{sand}$ . Very good correlations of Q and  $f_q$  with  $m_{sand}$  are observed, with  $r^2$  values of 416 0.72 and 0.83, respectively. This is consistent with our finding that  $f_q$  is systematically better 417 correlated to soil characteristics than Q (Sect. 3.2).

The pedotransfer functions derived from French soils tend to overestimate  $f_q$  for the Lu el al. (2007) soils, especially for the seven soils presenting  $m_{sand}/m_{SOM}$  values larger than 40. Note that Lu et al. (2007) obtained a similar result for coarse-textured soils with their model, which assumed  $Q = m_{sand}$ . For the three other soils, presenting  $m_{sand}/m_{SOM}$  values smaller than 40,  $f_q$ MAE values are given in Table 4. The best MAE score (0.071 m<sup>3</sup>m<sup>-3</sup>) is obtained for the  $m_{sand}*$ predictor of  $f_q$ .

424 These results are illustrated by Fig. 11 for the  $m_{\text{sand}}$  predictor of  $f_q$ . Figure 11 also shows the  $f_q$ 425 and  $\lambda_{sat}$  estimates obtained using specific coefficients in Eq. (12), based on the seven Lu et al. 426 (2007) soils presenting  $m_{\rm sand}/m_{\rm SOM}$  values larger than 40. These coefficients are given together 427 with the scores in Table 6. Table 6 also present these values for other predictors of  $f_q$ . It appears 428 that  $m_{\text{sand}}$  gives the best scores. The contrasting coefficient values between Table 6 and Table 3 429 (Chinese and French soils, respectively) illustrate the variability of the coefficients of 430 pedotransfer functions from one soil category to another, and the  $m_{\rm sand}/m_{\rm SOM}$  ratio seems to be a 431 good indicator of the validity of a given pedotransfer function.

On the other hand, the  $m_{\text{sand}}/m_{\text{SOM}}$  ratio is not a good predictor of  $f_q$  for the Lu et al. (2007) soils presenting  $m_{\text{sand}}/m_{\text{SOM}}$  values larger than 40, and  $r^2$  presents a small value of 0.40 (Table 6). This can be explained by the very large range of  $m_{\text{sand}}/m_{\text{SOM}}$  values for these soils (see Table S3.1). Using  $ln(m_{\text{sand}}/m_{\text{SOM}})$  instead of  $m_{\text{sand}}/m_{\text{SOM}}$  is a way to obtain a predictor linearly correlated to  $f_q$ . This is shown by Fig. 12 for the ten Lu et al. (2007) soils: the correlation is increased to a large extent ( $r^2 = 0.60$ ).

440 4.4. Can  $m_{\text{sand}}$ -based  $f_q$  pedotransfer functions be used across soil types ?

Given the results presented in Tables 3, 4, and 6, it can be concluded that  $m_{\text{sand}}$  is the best predictor of  $f_q$  across mineral soil types. The  $m_{\text{sand}}/m_{\text{SOM}}$  predictor is relevant for the mineral soils containing the largest amount of organic matter.

The results presented in this study suggest that the  $m_{sand}/m_{SOM}$  ratio can be used to differentiate temperate grassland soils containing a rather large amount of organic matter (3.7 <  $m_{sand}/m_{SOM}$  < 40) from soils containing less organic matter ( $m_{sand}/m_{SOM} > 40$ ). The  $m_{sand}$  predictor can be used in both cases, with the following  $a_0$  and  $a_1$  coefficient values in Eq. (12): 0.15 and 0.572 for  $m_{sand}/m_{SOM}$  ranging between 3.7 and 40 (Table 3), and 0.04 and 0.386 for  $m_{sand}/m_{SOM} > 40$  (Table 6), respectively.

Although the  $m_{\text{sand}}/m_{\text{SOM}}$  predictor gives the best  $r^2$  scores for the 14 grassland soils considered in this study, it seems more difficult to apply this predictor to other soils, as shown by the high MAE score (MAE = 0.135 m<sup>3</sup>m<sup>-3</sup>) for the corresponding Lu et al. (2007) soils in Table 4. Moreover, the scores are very sensitive to errors in the estimation of  $m_{\text{SOM}}$  as shown by Table 5. Although the  $m_{\text{sand}}$ \* predictor gives slightly better scores than  $m_{\text{sand}}$  (Table 4), the  $a_1$  coefficient in more sensitive to errors in  $C_{\text{hmin}}$  (Table 3), and the bootstrapping reveals large uncertainties in  $a_0$ and  $a_1$  values.

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462 4.5. Prospects for using soil temperature profiles

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Using standard soil moisture and soil temperature observations is a way to investigate soil thermal properties over a large variety of soils, as the access to such data is facilitated by online databases (Dorigo et al., 2013).

A limitation of the data used in this study, however, is that soil temperature observations ( $T_i$ ) are recorded with a resolution of  $\Delta T_i = 0.1$  °C only (see Sect. 2.1). This low resolution affects the accuracy of the soil thermal diffusivity estimates. In order to limit the impact of this effect, a data filtering technique is used (see Supplement 4) and  $D_h$  is retrieved with a precision of 18 %.

It can be noticed that if  $T_i$  data were recorded with a resolution of 0.03 °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. (S4.3). Therefore, one may recommend to revise the current practise of most observation networks consisting in recording soil temperature with a resolution of 0.1 °C only. More precision in the  $\lambda$  estimates would permit investigating other processes of heat transfer in the soil such as those related to water transport (Rutten, 2015).

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#### 479 **5.** Conclusions

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481 An attempt was made to use routine soil temperature and soil moisture observations of a network 482 of automatic weather stations to retrieve instantaneous values of the soil thermal conductivity at 483 a depth of 0.10 m. The data from the SMOSMANIA network, in southern France, are used. First, 484 the thermal diffusivity is derived from consecutive measurements of the soil temperature. The  $\lambda$ 485 values are then derived from the thermal diffusivity retrievals and from the volumetric heat 486 capacity calculated using measured soil properties. The relationship between the  $\lambda$  estimates and the measured soil moisture at a depth of 0.10 m permits the retrieval of  $\lambda_{sat}$  for 14 stations. The 487 488 Lu et al. (2007) empirical  $\lambda$  model is then used to retrieve the quartz volumetric content by 489 reverse modelling. A number of pedotransfer functions is proposed for volumetric fraction of 490 quartz, for the considered region in France. For the grassland soils examined in this study, the 491 ratio of sand to SOM fractions is the best predictor of  $f_q$ . A sensitivity study shows that omitting 492 gravels and the SOM information has a major impact on  $\lambda_{sat}$ . Eventually, an error propagation 493 analysis and a comparison with independent  $\lambda_{sat}$  data from Lu et al. (2007) show that the 494 gravimetric fraction of sand within soil solids, including gravels and SOM, is a good predictor of 495 the volumetric fraction of quartz when a larger variety of soil types is considered.

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506	References
500	iterer ences

508	Abu-Hamdeh, N. H., and Reeder, R. C.: Soil thermal conductivity: effects of density, moisture,
509	salt concentration, and organic matter, Soil Sci. Soc. Am. J., 64, 1285-1290, 2000.
510	Albergel, C., Rüdiger, C., Pellarin, T., Calvet, JC., Fritz, N., Froissard, F., Suquia, D., Petitpa,
511	A., Piguet, B., and Martin, E.: From near-surface to root-zone soil moisture using an
512	exponential filter: an assessment of the method based on in-situ observations and model
513	simulations, Hydrol. Earth Syst. Sci., 12, 1323–1337, 2008.
514	Albergel, C., Calvet, JC., de Rosnay, P., Balsamo, G., Wagner, W., Hasenauer, S., Naeimi, V.,
515	Martin, E., Bazile, E., Bouyssel, F., and Mahfouf, JF.: Cross-evaluation of modelled and
516	remotely sensed surface soil moisture with in situ data in southwestern France, Hydrol. Earth
517	Syst. Sci., 14, 2177–2191, doi:10.5194/hess-14-2177-2010, 2010.
518	Bristow, K. L., Kluitenberg, G. J., and Horton R.: Measurement of soil thermal properties with a
519	dual-probe heat-pulse technique, Soil Sci. Soc. Am. J., 58, 1288-1294,
520	doi:10.2136/sssaj1994.03615995005800050002x, 1994.
521	Bristow, K. L.: Measurement of thermal properties and water content of unsaturated sandy soil
522	using dual-probe heat-pulse probes, Agr. Forest Meteorol., 89, 75-84, 1998.
523	Calvet, JC., Bessemoulin, P., Noilhan, J., Berne, C., Braud, I., Courault, D., Fritz, N., Gonzalez-
524	Sosa, E., Goutorbe, JP., Haverkamp, R., Jaubert, G., Kergoat, L., Lachaud, G., Laurent, J
525	P., Mordelet, P., Olioso, A., Péris, P., Roujean, JL., Thony, JL., Tosca, C., Vauclin, M.,
526	Vignes, D.: MUREX: a land-surface field experiment to study the annual cycle of the energy
527	and water budgets, Ann. Geophys., 17, 838-854, 1999.
528	Calvet, JC., Fritz, N., Froissard, F., Suquia, D., Petitpa, A., and Piguet, B.: In situ soil moisture

529 observations for the CAL/VAL of SMOS: the SMOSMANIA network, International

530 Geoscience and Remote Sensing Symposium, IGARSS, Barcelona, Spain, 23–28 July 2007,

531 1196–1199, doi:10.1109/IGARSS.2007.4423019, 2007.

- 532 Chen, Y. Y., Yang, K., Tang, W., Qin, J., and Zhao, L.: Parameterizing soil organic carbon's
  533 impacts on soil porosity and thermal parameters for Eastern Tibet grasslands, Sci. China
- 534 Earth Sci., 55 (6), 1001–1011, doi:10.1007/s11430-012-4433-0, 2012.
- Côté, J. and Konrad, J.-M.: A generalized thermal conductivity model for soils and construction
  materials, Can. Geotech. J., 42, 443:458, doi:10.1139/T04-106, 2005.
- de Vries, D. A.: Thermal properties of soils, in W.R. Van Wijk (ed.), Physics of plant
  environment, pp. 210–235, North-Holland Publ. Co., Amsterdam, 1963.Dorigo, W. A.,
  Wagner, W., Hohensinn, R., Hahn, S., Paulik, C., Xaver, A., Gruber, A., Drusch, M,
  Mecklenburg, S., van Oevelen, P., Robock, A., and Jackson, T.: The International Soil
  Moisture Network: a data hosting facility for global in situ soil moisture measurements,
  Hydrol. Earth Syst. Sci., 15, 1675–1698, doi:10.5194/hess-15-1675-2011, 2011.
- 543 Draper, C., Mahfouf, J.-F., Calvet, J.-C., Martin, E., and Wagner, W.: Assimilation of ASCAT
- 544 near-surface soil moisture into the SIM hydrological model over France, Hydrol. Earth Syst.
- 545 Sci., 15, 3829–3841, doi:10.5194/hess-15-3829-2011, 2011.
- 546 Johansen, O.: Thermal conductivity of soils. Ph.D. thesis, University of Trondheim, 236 pp.,
- 547 Available from Universitetsbiblioteket i Trondheim, Høgskoleringen 1, 7034 Trondheim,
- Norway, a translation is available at: http://www.dtic.mil/dtic/tr/fulltext/u2/a044002.pdf (last
  access January 2016), 1975.
- Lu, S., Ren, T., Gong, Y., and Horton, R.: An improved model for predicting soil thermal
  conductivity from water content at room temperature, Soil Sci. Soc. Am. J., 71, 8-14,
  doi:10.2136/sssai2006.0041, 2007.
- 553 Nachtergaele, F., van Velthuize, H., Verelst, L., Wiberg, D., Batjes, N., Dijkshoorn, K., van
- 554 Engelen, V., Fischer, G., Jones, A., Montanarella, L., Petri, M., Prieler, S., Teixeira, E., and

- 555 Shi, X.: Harmonized World Soil Database, Version 1.2, FAO/IIASA/ISRIC/ISS-CAS/JRC,
- Laxenburg, 556 FAO. Rome. Italy and IIASA. available Austria. at: 557 http://webarchive.iiasa.ac.at/Research/LUC/External-World-soil-
- 558 database/HWSD Documentation.pdf (last access January 2016), 2012.
- 559 Parlange, M. B., Cahill, A. T., Nielsen, D. R., Hopmans, J. W., and Wendroth, O.: Review of 560 heat and water movement in field soils, Soil Till. Res., 47, 5-10, 1998.
- 561 Parrens, M., Zakharova, E., Lafont, S., Calvet, J.-C., Kerr, Y., Wagner, W., and Wigneron, J.-P.:
- 562 Comparing soil moisture retrievals from SMOS and ASCAT over France, Hydrol. Earth Syst.
- 563 Sci., 16, 423-440, doi:10.5194/hess-16-423-2012, 2012.
- Peters-Lidard, C.D., Blackburn, E., Liang, X., and Wood, E.F.: The effect of soil thermal 564 conductivity parameterization on surface energy fluxes and temperatures, J. Atmos. Sci., 55, 565 566 1209-1224, 1998.
- Rutten, M. M.: Moisture in the topsoil: From large-scale observations to small-scale process 567 understanding, PhD Thesis, Delft university of Technology, doi:10.4233/uuid:89e13a16-568 569 b456-4692-92f0-7a40ada82451,
- 570 http://repository.tudelft.nl/view/ir/uuid:89e13a16-b456-4692-92f0-7a40ada82451/ (last

available

- 571 access: January 2016), 2015.
- 572
- 573 Schelde, K., Thomsen, A., Heidmann, T., Schjonning, P., and Jansson, P.-E.: Diurnal fluctuations 574 of water and heat flows in a bare soil, Water Resour. Res., 34, 11, 2919-2929, 1998.
- 575 Schönenberger, J., Momose, T., Wagner, B., Leong, W. H., and Tarnawski, V. R.: Canadian field
- 576 soils I. Mineral composition by XRD/XRF measurements, Int. J. Thermophys., 33, 342–362,
- 577 doi:10.1007/s10765-011-1142-4, 2012.

at:

- 578 Tarara, J.M., and J.M. Ham: Measuring soil water content in the laboratory and field with dual-579 probe heat-capacity sensors, Agron. J., 89, 535–542, 1997.
- Tarnawski, V. R., McCombie, M. L., Leong, W. H., Wagner, B., Momose, T., and
  Schönenberger J.: Canadian field soils II. Modeling of quartz occurrence, Int. J.
  Thermophys., 33, 843–863, doi:10.1007/s10765-012-1184-2, 2012.
- Tarnawski, V. R., Momose, T., and Leong, W. H.: Assessing the impact of quartz content on the
  prediction of soil thermal conductivity, Géotechnique, 59, 4, 331–338, doi:
  10.1680/geot.2009.59.4.331, 2009.
- Yang, K., Koike, T., Ye, B., and Bastidas, L.: Inverse analysis of the role of soil vertical
  heterogeneity in controlling surface soil state and energy partition, J. Geophys. Res., 110,
  D08101, 15 pp., doi:10.1029/2004JD005500, 2005.
- Zhang, X., Heitman, J., Horton, R., and Ren, T.: Measuring near-surface soil thermal properties
  with the heat-pulse method: correction of ambient temperature and soil–air interface effects,
- 591 Soil Sci. Soc. Am. J., 78, 1575–1583, doi:10.2136/sssaj2014.01.0014, 2014.

592 **Table 1** – Soil characteristics at 10 cm for the 21 stations of the SMOSMANIA network. 593 Porosity values are derived from Eq. (1). Solid fraction values higher than 0.3 are in bold. The 594 stations are listed from West to East (from top to bottom).  $\rho_d$ ,  $\theta_{sat}$ , *f*, and *m*, stand for soil bulk 595 density, porosity, volumetric fractions, and gravimetric fractions, respectively.

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Soil	$\rho_{\rm d}$ (kg m <sup>-3</sup> )	$\theta_{\rm sat}$ (m <sup>3</sup> m <sup>-3</sup> )	$f_{\rm sand}$ (m <sup>3</sup> m <sup>-3</sup>	$f_{clay}$ ) (m <sup>3</sup> m <sup>-3</sup> )	$f_{\text{silt}}$ ) (m <sup>3</sup> m <sup>-3</sup>	$f_{\text{gravel}}$ ) (m <sup>3</sup> m <sup>-3</sup> )	$f_{\text{SOM}}$ (m <sup>3</sup> m <sup>-3</sup> )	$m_{\rm sand}$ ) (kg kg <sup>-1</sup> )	$m_{\text{clay}}$ (kg kg <sup>-1</sup>	$m_{\rm silt}$ ) (kg kg <sup>-1</sup> )	m <sub>gravel</sub> (kg kg <sup>-1</sup> )	<i>m</i> <sub>SOM</sub> (kg kg <sup>-1</sup> )
SBR	1680	0.352	0.576	0.026	0.013	0.002	0.032	0.911	0.041	0.020	0.003	0.024
URG	1365	0.474	0.076	0.078	0.341	0.005	0.025	0.149	0.153	0.665	0.009	0.024
CRD	1435	0.438	0.457	0.027	0.033	0.000	0.045	0.848	0.051	0.060	0.000	0.041
PRG	1476	0.431	0.051	0.138	0.138	0.214	0.028	0.092	0.250	0.248	0.385	0.025
CDM	1522	0.413	0.073	0.241	0.231	0.012	0.030	0.128	0.422	0.404	0.020	0.026
LHS	1500	0.416	0.102	0.202	0.189	0.051	0.039	0.181	0.359	0.335	0.091	0.034
SVN	1453	0.445	0.127	0.073	0.176	0.162	0.017	0.233	0.133	0.322	0.296	0.015
MNT	1444	0.447	0.135	0.066	0.230	0.102	0.020	0.248	0.121	0.424	0.188	0.018
SFL	1533	0.413	0.127	0.071	0.118	0.250	0.021	0.221	0.123	0.205	0.434	0.018
MTM	1540	0.405	0.110	0.081	0.076	0.297	0.032	0.189	0.140	0.131	0.512	0.027
LZC	1498	0.429	0.129	0.066	0.068	0.292	0.015	0.229	0.117	0.121	0.519	0.013
NBN	1545	0.401	0.063	0.135	0.075	0.290	0.035	0.109	0.232	0.130	0.499	0.030
PZN	1311	0.495	0.222	0.074	0.131	0.054	0.023	0.450	0.151	0.266	0.111	0.023
PRD	1317	0.494	0.038	0.052	0.069	0.326	0.021	0.076	0.105	0.139	0.659	0.021
LGC	1496	0.428	0.253	0.044	0.042	0.214	0.019	0.451	0.078	0.074	0.380	0.017
MZN	1104	0.560	0.212	0.037	0.045	0.097	0.049	0.510	0.089	0.109	0.234	0.057
VLV	1274	0.506	0.294	0.054	0.086	0.031	0.029	0.614	0.112	0.179	0.064	0.030
BRN	1630	0.379	0.105	0.009	0.016	0.474	0.016	0.171	0.015	0.027	0.774	0.013
MJN	1276	0.506	0.064	0.029	0.056	0.317	0.028	0.133	0.060	0.118	0.661	0.029
BRZ	1280	0.508	0.097	0.074	0.109	0.190	0.020	0.202	0.154	0.228	0.396	0.021
CBR	1310	0.501	0.120	0.057	0.068	0.241	0.013	0.243	0.116	0.139	0.489	0.013

**Table 2** – Thermal properties of 14 grassland soils in southern France:  $\lambda_{sat}$ ,  $f_q$  and Q retrievals 599 using the  $\lambda$  model (Eqs. (7)-(9) and Eq. (10), respectively) for degree of saturation values higher 600 than 0.4, together with the minimized RMSD between the simulated and observed  $\lambda$  values, and 601 the number of used  $\lambda$  observations (*n*). The soils are sorted from the largest to the smallest ratio 602 of  $m_{sand}$  to  $m_{SOM}$ .

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Soil	$\lambda_{\text{sat}}$ (Wm <sup>-1</sup> K <sup>-1</sup> )	RMSD (Wm <sup>-1</sup> K <sup>-1</sup> )	n	$f_{q}$ (m <sup>3</sup> m <sup>-3</sup> )	Q (kg kg <sup>-1</sup> )	m <sub>sand</sub> m <sub>SOM</sub>
SBR	2.80	0.255	6	0.62	0.96	37.2
LGC	2.07	0.311	20	0.44	0.77	26.6
CBR	1.92	0.156	20	0.44	0.88	18.4
LZC	1.71	0.107	20	0.29	0.51	17.3
SVN	1.78	0.163	20	0.34	0.61	15.4
MNT	1.96	0.058	20	0.42	0.76	13.8
BRN	1.71	0.131	20	0.25	0.40	13.5
SFL	1.57	0.134	20	0.22	0.37	12.5
MTM	1.52	0.095	20	0.21	0.35	7.0
URG	1.37	0.066	20	0.05	0.10	6.2
LHS	1.57	0.136	20	0.26	0.45	5.3
CDM	1.82	0.086	20	0.26	0.44	5.0
PRG	1.65	0.086	20	0.18	0.32	3.7
PRD	1.26	0.176	20	0.14	0.28	3.7

609 **Table 3** – Coefficients of four pedotransfer functions of  $f_q$  for 14 soils of this study, together 610 with indicators of the coefficient uncertainty, derived by bootstrapping and by perturbing the 611 volumetric heat capacity of soil minerals ( $C_{\text{hmin}}$ ). The best predictor is in bold.

	Coefficient	ts for 14 soils	Confide	nce interval	Impact of a change of		
Predictor of $f_q$			from bo	otstrapping	$\pm 0.08 \times 10^{6} \text{ J m}^{-3} \text{ K}^{-1}$ in		
					$C_{ m hmin}$		
	$a_0$	$a_1$	$a_0$	$a_1$	$a_0$	$a_1$	
$m_{\rm sand} / m_{\rm SOM}$	0.12	0.0134	[0.10,0.14]	[0.012,0.014]	[0.11,0.13]	[0.013,0.013]	
m <sub>sand</sub> *	0.08	0.944	[0.00,0.11]	[0.85,1.40]	[0.07,0.09]	[0.919,0.966]	
<i>m</i> <sub>sand</sub>	0.15	0.572	[0.08,0.17]	[0.54,0.94]	[0.14,0.17]	[0.55,0.56]	
$1 -  heta_{sat} - f_{sand}$	0.73	-1.020	[0.71,0.89]	[-1.38, -0.99]	[0.70,0.73]	[-1.00, -0.99]	
612 (*) only $m_{\text{cond}}$ val	lues smaller t	han () 6 kg kg <sup>-1</sup>	are used in th	ne regression			

612 (\*) only  $m_{\text{sand}}$  values smaller than 0.6 kg kg<sup>-1</sup> are used in the regression

**Table 4** – Scores of four pedotransfer functions of  $f_q$  for 14 soils of this study, together with the 614 scores obtained by bootstrapping, without the sandy SBR soil. The MAE score of these 615 pedotransfer functions for three Chinese soils of Lu et al. (2007) for which  $m_{sand}/m_{SOM} < 40$  is 616 given. The best predictor and the best scores are in bold.

	R	egression s	cores	Bo	ootstrap so	cores	Sco	res withou	ıt SBR
Predictor of $f_q$						(and MAE for 3 Lu soils)			
	$r^2$	RMSD	MAE	$r^2$	RMSD	MAE	$r^2$	RMSD	MAE
		$(m^3m^{-3})$	$(m^3m^{-3})$		$(m^3m^{-3})$	$(m^3m^{-3})$		$(m^3m^{-3})$	$(m^3m^{-3})$
$m_{\rm sand} / m_{\rm SOM}$	0.77	0.067	0.053	0.72	0.074	0.059	0.62	0.070	0.057 ( <i>0.135</i> )
<i>m</i> <sub>sand</sub> *	0.74	0.072	0.052	0.67	0.126	0.100	0.56	0.075	0.056 (0.071)
<i>m</i> <sub>sand</sub>	0.67	0.081	0.060	0.56	0.121	0.084	0.56	0.075	<b>0.056</b> (0.086)
$1 - \theta_{\rm sat} - f_{\rm sand}$	0.65	0.084	0.064	0.56	0.102	0.079	0.45	0.084	0.061 ( <i>0.158</i> )

617 (\*) only  $m_{sand}$  values smaller than 0.6 kg kg<sup>-1</sup> are used in the regression

623	<b>Table 5</b> – Ability of the Eqs. (10)-(13) empirical model to estimate $\lambda_{sat}$ values for 14 soils and
624	impact of changes in gravel and SOM volumetric content: $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$ and $f_{\text{SOM}} = 0.013$
625	$m^3m^{-3}$ (the smallest $f_{SOM}$ value, observed for CBR). $r^2$ values smaller than 0.60, RMSD values
626	higher than 0.20 $\text{Wm}^{-1}\text{K}^{-1}$ , and mean bias values higher (smaller) than +0.10 (-0.10) are in bold.

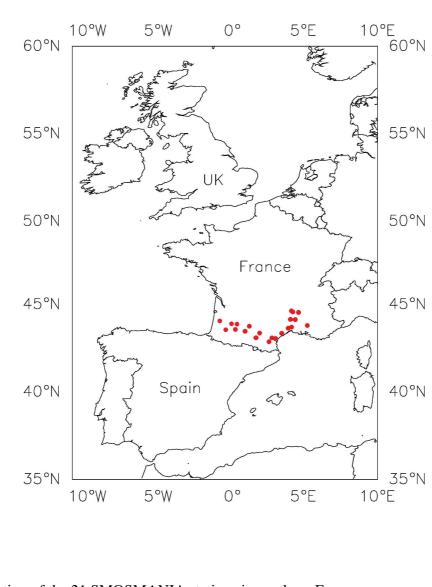
Model configuration	Predictor of $f_q$	$r^2$	RMSD (Wm <sup>-1</sup> K <sup>-1</sup> )	Mean bias (Wm <sup>-1</sup> K <sup>-1</sup> )	
Model using $\theta_{sat}$ observations	$m_{\rm sand} / m_{\rm SOM}$	0.86	0.14	+0.01	
	$m_{\rm sand}*$	0.83	0.15	-0.01	
	m <sub>sand</sub>	0.81	0.16	-0.03	
	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.82	0.16	-0.03	
Full model using $\theta_{satMOD}$ (Eqs. (13))		0.85	0.14	+0.03	
	$m_{ m sand} / m_{ m SOM} \ m_{ m sand}^{st}$	0.85	0.14	+0.03 -0.03	
		0.83	0.14		
	$m_{ ext{sand}} \ 1 -  heta_{ ext{sat}} - f_{ ext{sand}}$	0.84	0.16	-0.03 -0.02	
same with:	$m_{\rm sand} / m_{\rm SOM}$	0.57	0.35	+0.20	
$f_{\rm SOM} = 0.013 \text{ m}^3 \text{m}^{-3}$	$m_{\rm sand}*$	0.83	0.15	+0.00	
J DOWN	$m_{\rm sand}$	0.81	0.16	-0.02	
	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.83	0.15	-0.02	
same with:	$m_{\rm sand} / m_{\rm SOM}$	0.87	0.19	-0.12	
$f_{\rm gravel} = 0 \ {\rm m}^3 {\rm m}^{-3}$	$m_{\rm sand}*$	0.70	0.23	+0.11	
	$m_{\rm sand}$	0.79	0.17	+0.04	
	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.81	0.17	+0.05	
same with:	$m_{\rm sand} / m_{\rm SOM}$	0.63	0.31	+0.16	
$f_{\rm SOM} = 0.013 \text{ m}^3 \text{m}^{-3}$	$m_{\rm sand}*$	0.52	0.36	+0.24	
and $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$	$m_{\rm sand}$	0.59	0.29	+0.16	
,	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.70	0.25	+0.16	

(\*) only  $m_{sand}$  values smaller than 0.6 kg kg<sup>-1</sup> are used in the regression

	Regr	Regression scores				
Predictor of $f_q$	for 7 Lu soils with $m_{\rm sand}/m_{\rm SOM} > 40$			Coefficients		
		(p-value)	$(m^3m^{-3})$	$(m^3m^{-3})$	$a_0$	$a_1$
$m_{\rm sand} / m_{\rm SOM}$	0.40 (0.13)	0.089	0.075	0.20	0.000148	
m <sub>sand</sub> *	0.82 (0.005)	0.073	0.054	0.07	0.425	
<i>M</i> sand	0.82 (0.005)	0.048	0.042	0.04	0.386	
$1 - \theta_{\rm sat} - f_{\rm sand}$	0.81 ( <i>0.006</i> )	0.050	0.043	0.44	-0.814	

**Table 6** – Pedotransfer functions of  $f_q$  for 7 soils of Lu et al. (2007) with  $m_{\text{sand}}/m_{\text{SOM}} > 40$ . The best predictor and the best scores are in bold.

(\*) only  $m_{sand}$  values smaller than 0.6 kg kg<sup>-1</sup> are used in the regression

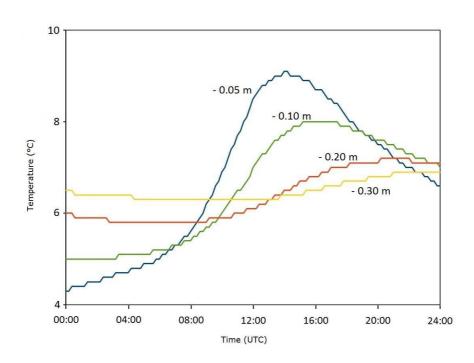


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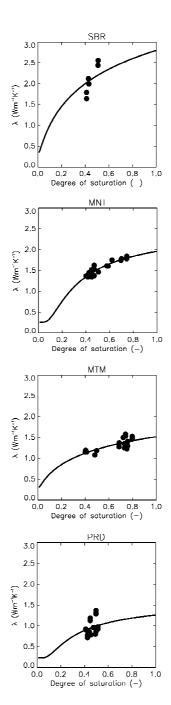
Fig. 1 – Location of the 21 SMOSMANIA stations in southern France.

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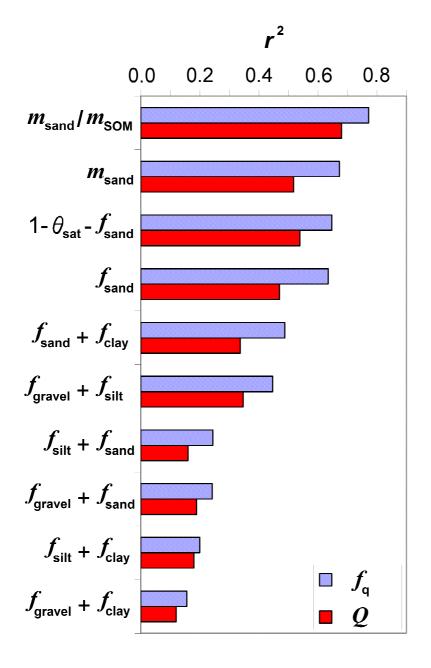




**Fig. 2** – Soil temperature measured at the Saint-Félix-de-Lauragais (SFL) station on 23 February 661 2015, at depths of 0.05, 0.10, 0.20, and 0.30 m. Levelling is due to the low resolution of the 662 temperature records  $(0.1^{\circ}C)$ .

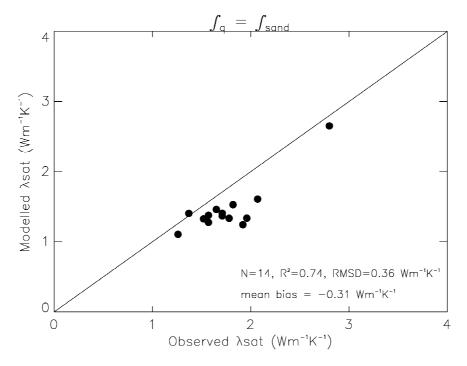


**Fig. 3** – Retrieved  $\lambda$  values (dark dots) vs. the observed degree of saturation of the soil, at a 668 depth of 0.10 m, for (from top to bottom) Sabres (SBR), Montaut (MNT), Mouthoumet (MTM), 669 and Prades-le-Lez (PRD), together with simulated  $\lambda$  values from dry to wet conditions (dark 670 lines).

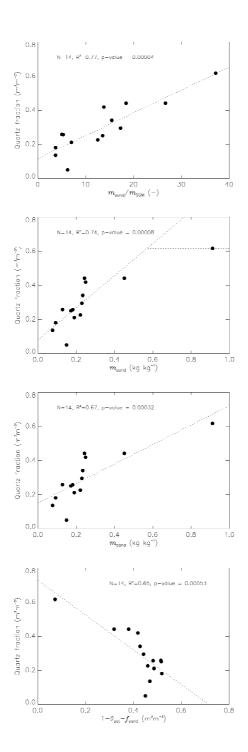




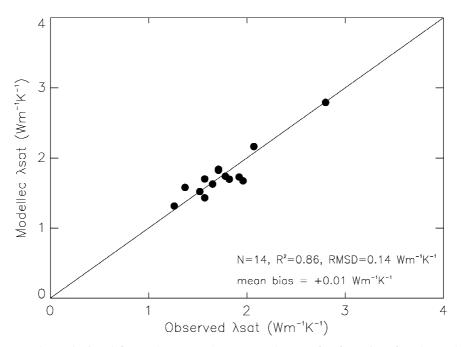
**Fig. 4** – Fraction of variance  $(r^2)$  of gravimetric and volumetric fraction of quartz (Q and  $f_q$ , red 674 and blue bars, respectively) explained by various predictors. 675



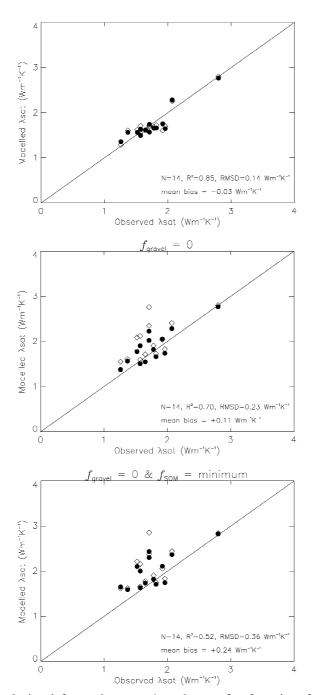
676 677 Fig. 5 –  $\lambda_{satMOD}$  values derived from volumetric quartz fractions  $f_q$  assumed equal to  $f_{sand}$ , using 678 679 observed  $\theta_{sat}$  values, vs.  $\lambda_{sat}$  retrievals.



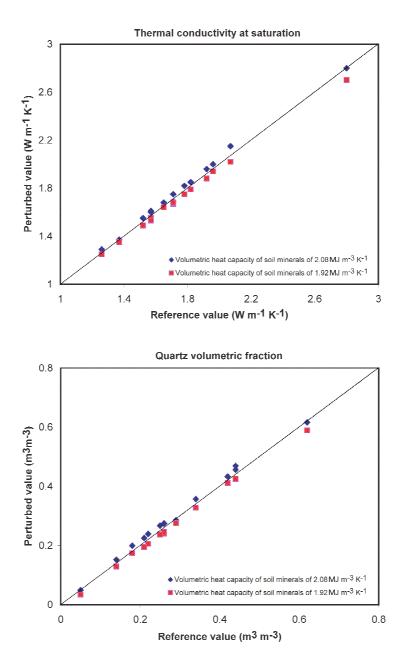
**Fig. 6** – Pedotransfer functions for quartz:  $f_q$  retrievals (dark dots) vs. the four predictors of  $f_q$  given in Table 3. The modelled  $f_q$  values are represented by the dashed lines. 



684 Fig. 7 –  $\lambda_{satMOD}$  values derived from the  $m_{sand}$  /  $m_{SOM}$  pedotransfer function for the volumetric quartz fractions, using observed  $\theta_{sat}$  values, vs.  $\lambda_{sat}$  retrievals. 

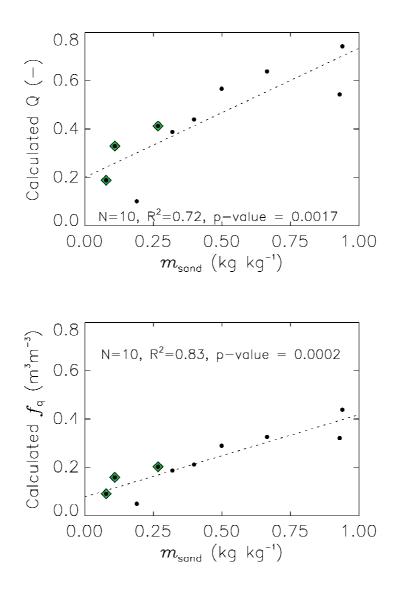


**Fig. 8** –  $\lambda_{satMOD}$  values derived from the  $m_{sand}^*$  pedotransfer function for the volumetric quartz fractions, using  $\theta_{\text{satMOD}}$  (Eqs. (13)) or the observed  $\theta_{\text{sat}}$  (dark dots and opened diamonds, respectively), vs.  $\lambda_{\text{sat}}$  retrievals: (top) full model, (middle)  $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$ , (bottom)  $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$  and  $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$ . Scores are given for the  $\theta_{\text{satMOD}}$  configuration. 





**Fig. 9** – Impact of using values of  $C_{\text{hmin}} = 1.92 \text{ MJ m}^{-3} \text{ K}^{-1}$  and  $C_{\text{hmin}} = 2.08 \text{ MJ m}^{-3} \text{ K}^{-1}$  instead of *C*<sub>hmin</sub> = 2.0 MJ m<sup>-3</sup> K<sup>-1</sup> on (top) the retrieved  $\lambda_{\text{sat}}$ , (bottom) the volumetric fraction of quartz.



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**Fig. 10** – Gravimetric and volumetric fraction of quartz (top and bottom, respectively) derived from the  $\lambda_{sat}$  observations of Lu et al. (2007) for 10 soils given by Tarnawski et al. (2009), vs. the gravimetric fraction of sand  $m_{sand}$ . The three soils for which  $m_{sand}/m_{SOM} < 40$  are indicated by green diamonds. The dashed lines represent the regression equations based on all soils: Q = 0.20 $+ 0.54 m_{sand}$  and  $f_q = 0.08 + 0.34 m_{sand}$ .

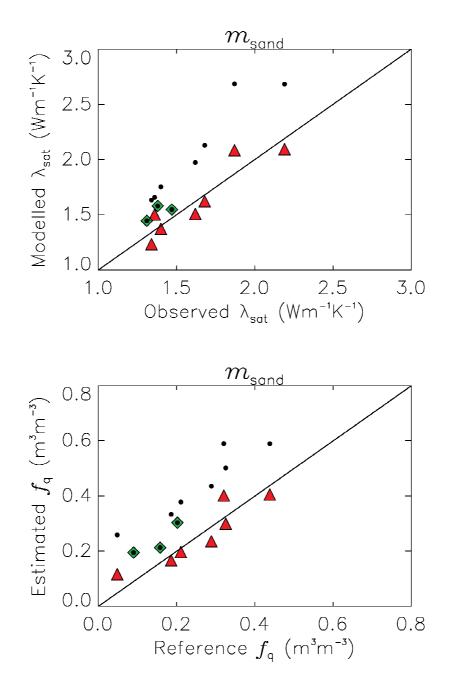


Fig. 11 – Estimated  $\lambda_{sat}$  and volumetric fraction of quartz  $f_q$  (top and bottom, respectively) vs. values derived from the  $\lambda_{sat}$  observations of Lu et al. (2007) given by Tarnawski et al. (2009) for 10 Chinese soils, using the gravimetric fraction of sand  $m_{sand}$  as a predictor of  $f_q$ . Dark dots correspond to the estimations obtained using the  $m_{sand}$  pedotransfer function for southern France and the three soils for which  $m_{sand}/m_{SOM} < 40$  are indicated by green diamonds. Red triangles correspond to the estimations obtained using the  $m_{sand}$  pedotransfer function for the seven soils for which  $m_{sand}/m_{SOM} > 40$ .

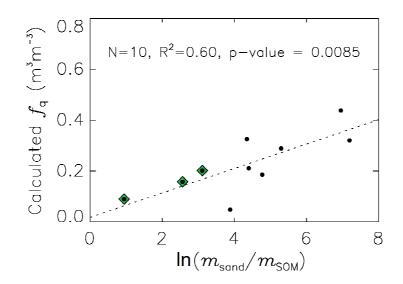




Fig. 12 – Volumetric fraction of quartz derived from the  $\lambda_{sat}$  observations of Lu et al. (2007) given by Tarnawski et al. (2009), vs. the logarithm of the  $m_{sand} / m_{SOM}$  ratio. The three soils for which  $m_{sand}/m_{SOM} < 40$  are indicated by green diamonds. The dashed line represents the regression equation:  $f_q = 0.02 + 0.048 \ln(m_{sand}/m_{SOM})$ .

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