Calvet el al. (2015), www.soil-discuss.net/2/737/2015/

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

13 January 2016.

Dear Prof. Nunzio Romano,

Please find enclosed a point by point response to the reviewers' comments, together with changes in the revised version of our work. In response to the reviewers' comments, we implemented a new data analysis procedure able to sort out flawed soil thermal conductivity estimates. This greatly improved our results and we are confident in the new retrieved values of volumetric fraction of quartz. We used the data published by Lu et al. (2007) to validate and discuss our results. For the sake of consistency, the empirical Lu et al. (2007) model was used. We have endeavoured to characterize the impact of uncertainties in data and models. We extensively revised the text, added new Figures, Tables, and Supplements. The Title and Abstract were rewritten.

Moreover, we made the soil profile data available on the web and the Supplements provide all the information needed to reproduce our calculations.

Sincerely,

Jean-Christophe Calvet and co-authors

Calvet el al. (2015), www.soil-discuss.net/2/737/2015/

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

Response to Reviewer #1 and changes in the revised version of the paper (X. Xiao, xinhua.xiao@aamu.edu; xiaoxinhua2009@gmail.com)

The authors thank Dr. Xinhua Xiao (NC State University Soil Physics) for her review of the manuscript and for the fruitful comments.

1.1 [Accuracy of predicative λ models highly depends on accurate estimation of λ sat and q, which has been oversimplified as sand fraction. It is interesting and important to predict q and λ sat in λ models using data of soil texture and gravel and SOM and to further examine their impacts on λ models. The methodology in this work to address the research question is appropriate. Discussion of model applicability is covered. The new pedotransfer functions for λ sat and q derived from their original data will add good contribution to the literature. I however have major concerns about the presentation/organization of this paper that I feel in some sections focus is lacking and/or reorganization needed. Better justification of adopting some key empirical models and more relevant discussion are also desired.]

RESPONSE 1.1

Many thanks for these positive comments. We will do our best to account for your remarks in a revised version of the manuscript.

Additional comments

In response to the reviewers' comments, we have revised our approach. The λ retrievals influenced by heterogeneities in soil properties are now sorted out. As a result, we now obtain realistic λ_{sat} values for 14 soils. We improved the assessment of uncertainties on the pedotranfer function for quartz volumetric fraction:

- a variety of pedotransfer functions is now proposed, not only one
- a confidence interval for the coefficients of pedotransfer functions is given
- the impact of errors on the volumetric heat capacity of soil minerals is assessed
- the data from Lu et al. (2007) are used as an independent benchmark to verify the obtained pedotransfer functions.

In order to clarify the definition of symbols, the volumetric fraction of quartz is now written as " f_q " (instead of "q").

Finally, the Kersten number model of Lu et al. (2007) is now used instead of the Yang et al. (2005) model.

1.2 [On obtaining site/station specific λ sat and q values. Equations 7-11 are the core functions for authors to enable retrieval of the site/station-specific λ sat (and q value accordingly) by parameter fitting via reverse modeling. I think these equations/models (specifically Lu et al 2007 and Yang et al 2005) should to some extent be justified why they were chosen as opposed to other alternative equations in the literatures.]

RESPONSE 1.2

Yes, two key equations are used for λ_{dry} and for K_e (Eqs. (7) and (9), respectively).

For $\lambda_{\rm dry}$ we used the Lu et al. (2007) parameterization. Figure R1.1 shows that this parameterization produces larger $\lambda_{\rm dry}$ values than the $\lambda_{\rm dry}$ estimates derived from Côté and Konrad (2005) for mineral soils. We checked that using Côté and Konrad (2005) instead of Lu et al. (2007) has a very limited impact on $\lambda_{\rm sat}$ and q retrievals ($\leq 0.005~{\rm Wm}^{-1}{\rm K}^{-1}$ and $\leq 0.01~{\rm m}^{-3}{\rm m}^{-3}$, respectively).

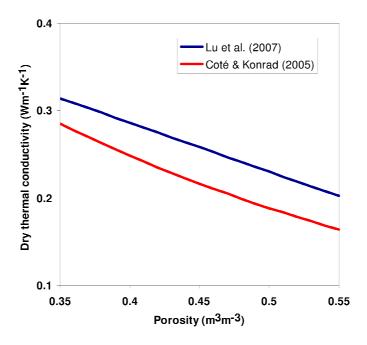


Figure R1.1 - Modelled λ_{dry} for the range of porosity values encountered in this study, using Lu et al. (2007) and Côté and Konrad (2005).

In the first version of this work, we used the Kersten number calculation used by Yang et al. (2005). Figure R1.2 shows the resulting K_e value, together the K_e value obtained using the Lu et al. (2007) model for fine and coarse soils. It can be seen that most differences between these models occur for S_d values < 0.4. Since we only use λ retrievals for S_d values > 0.4, the impact of the uncertainties in the determination of K_e is limited. However, using Lu et al. (2007) instead of Yang et al. (2005) tends to produce smaller values of λ_{sat} and f_q retrievals, as shown by Figs. R1.3 and R1.4. The impact of the Kersten number calculation will be discussed in the final version of this work.

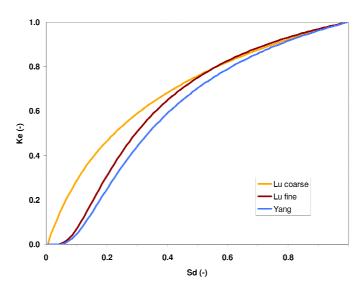


Figure R1.2 - Kersten number vs. degree of saturation as modelled by Lu et al. (2007) for coarse and fine soils, and as modelled by Yang et al. (2005).

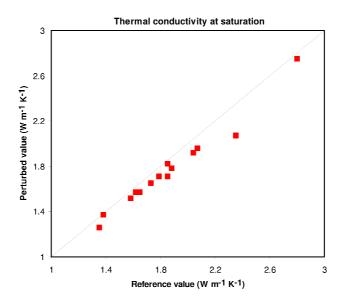


Figure R1.3 - λ_{sat} retrievals using the Kersten number as modelled by Lu et al. (2007) vs. those using the Kersten number as modelled by Yang et al. (2005).

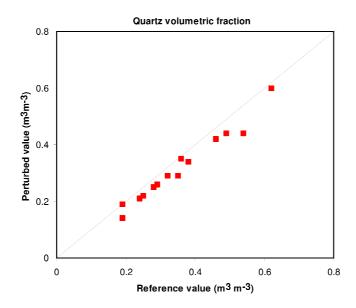


Figure R1.4 - As in Fig. R1.3, except for f_0 retrievals.

CHANGES 1.2 (Sect. 2.5)

In this study, the formula recommended by Lu et al. (2007) is used:

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

with $\alpha = 0.96$ for $Mn_{\rm sand} \ge 0.4$ kg kg⁻¹, $\alpha = 0.27$ for $Mn_{\rm sand} < 0.4$ kg kg⁻¹, and

$$S_d = \theta/\theta_{sat}$$
 (9).

 $Mn_{\rm sand}$ represents the sand mass fraction of fine earth minerals (values are given in Supplement 1).

Following Peters-Lidard et al. (1998), λ_{other} is taken as 2.0 Wm⁻¹K⁻¹ for soils with Mn_{sand} > 0.2 kg kg⁻¹, and 3.0 Wm⁻¹K⁻¹ otherwise. In this study, Mn_{sand} > 0.2 kg kg⁻¹ for all soils except for URG, PRG, and CDM.

1.3 [On discussion. First, the pedotransfer function for q (and thus λ sat) was evaluated with 11 stations/sites in this study but not tested. One alternative to be discussed is to

divide the 11 stations that some are used for model development and others for testing its predictive/generalization power.]

RESPONSE 1.3

Yes, this is a very good point. In order to address this issue, we have used a simple bootstrapping resampling technique consisting in calculating a new estimate of f_q for each soil using the pedotransfer function obtained without using this specific soil. Gathering these new f_q estimates, one can calculate new scores with respect to the retrieved f_q values. Also, this method provides a range of possible values of the coefficients of the pedotransfer function and permits assessing the influence of a given f_q retrieval on the final result.

These additional scores will be published in the final version of this work.

CHANGES 1.3

New Tables were added in order to list the potential pedotransfer functions and the associated scores (see below). The bootstrapping is described in Sect. 2.7.

Table 3 – Coefficients of four pedotransfer functions of f_q for 14 soils of this study, together with indicators of the coefficient uncertainty derived by bootstrapping and by perturbing the volumetric heat capacity of soil minerals (C_{hmin}).

	Coefficients for 14 soils		Confider	nce interval	Impact of a change of			
Predictor of $f_{ m q}$			from boo	otstrapping	$\pm 0.08 \text{ MJ m}^{-3} \text{ K}^{-1} \text{ in } C_{\text{hmin}}$			
	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]		
$m_{ m sand}*$	0.08	0.944	[0.00,0.11]	[0.85,1.40]	[0.07,0.09]	[0.919,0.966]		
$m_{ m sand}$	0.15	0.572	[0.08,0.17]	[0.54,0.94]	[0.14,0.17]	[0.55,0.56]		
$1-\theta_{\rm sat}-f_{\rm sand}$	0.73	-1.020	[0.71,0.89]	[-1.38,-0.99]	[0.70,0.73]	[-1.00,-0.99]		

^(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

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

	Regression scores		В	ootstrap so	cores	Scores without SBR				
Predictor of $f_{ m q}$							(and N	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	
									(0.135)	
$m_{ m sand}^*$	0.74	0.072	0.052	0.67	0.126	0.100	0.56	0.075	0.056	
									(0.071)	
	0.47	0.001	0.050	0.75	0.404	0.004	0.75	0.055	0.0=<	
m_{sand}	0.67	0.081	0.060	0.56	0.121	0.084	0.56	0.075	0.056	
									(0.086)	
1 0 0	0.65	0.004	0.064	0.56	0.102	0.070	0.45	0.004	0.061	
$1-\theta_{\rm sat}-f_{ m sand}$	0.65	0.084	0.064	0.56	0.102	0.079	0.45	0.084	0.061	
									(0.158)	

^(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

1.4 [Second, the impact of q on λ prediction actually has been studied in Tarnawski et al 2009, in which q was shown mostly linearly dependent on coarse fraction including sand and gravel. Authors recognized that work in this paper yet need to perform enough comparisons with that work and/or other related previous work in the literatures.]

RESPONSE 1.4

Yes. It is interesting to test the statistical relationships we get between f_q retrievals and soil characteristics using the independent data from Lu et al. (2007) and Tarnawski et al. (2009). We checked that the pedotransfer function(s) we get from our observations produce λ_{sat} values close to those observed for the fine-textured Lu soils. For coarse-textured soils, our pedotransfer function(s) tend(s) to overestimate λ_{sat} values. Note that Lu et al. (2007) obtained a similar result with their model, which assumes that $f_q = (1 - \theta_{\text{sat}}) \times m_{\text{SAND}}$. It must be noted that most of these soils contain very little organic matter and consisted of reassembled sieved soil samples, while our data concern undisturbed soils.

REFERENCES:

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/sssaj2006.0041, 2007.

Tarnawski V. R., T. Momose, W. H. Leong, 2009: 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.

CHANGES 1.4 (Sect. 4.3)

The characteristics of ten Chinese soils used by Lu et al. (2007) to investigate soil thermal conductivity are given in Table S1 (Supplement). We used three soils from the Lu et al. (2007) data to validate our approach: Silty clay loam 8, Silt loam 6, Silt loam 5. These soils were used as they present $m_{\text{sand}}/m_{\text{SOM}}$ values lower than 40, as the soils considered in this study. The other seven soils were used to propose alternative coefficient values for contrasting soil characteristics ($m_{\text{sand}}/m_{\text{SOM}} > 40$).

We derived gravimetric and volumetric fraction of quartz (Q and f_q , respectively) from the λ_{sat} observations of Lu et al. (2007). Figure 10 shows that f_q correlates to m_{sand} better than Q. Similar results are found for other predictors. This is consistent with the results we obtained

for 14 French soils: pedotransfer functions for quartz present systematically better scores using f_q instead of Q, as shown by Fig. 5.

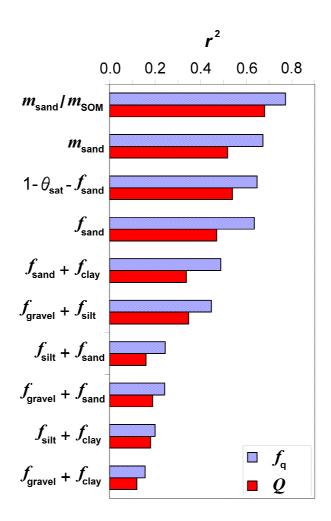


Figure 5 - Fraction of variance (r^2) of gravimetric and volumetric fraction of quartz $(Q \text{ and } f_q)$ red and blue bars, respectively) explained by various predictors.

Table S3.1 – Soil characteristics of ten Chinese soils of Lu et al. (2007). ρ_d , θ_{sat} , f, and m, stand for soil bulk density, porosity, volumetric fractions, and gravimetric fractions, respectively. λ_{sat} experimental values are derived from Table 3 in Tarnawski et al. (2009). Soil density is derived from porosity values inverting Eq. (1). The soils are sorted from the largest to the smallest ratio of m_{sand} to m_{som} . The ratio values smaller than 40 are in bold.

Lu et al. (2007) soils	* *Sat	ρ _d (kg m ⁻³)	θ_{sat} (m ³ m ⁻³)	f_{sand} (m ³ m ⁻³)	f_{clay} $(\text{m}^3\text{m}^{-3})$	f_{silt} (m ³ m ⁻³)	f_{SOM} (m ³ m ⁻³)	$m_{\rm sand}$ (kg kg ⁻¹)	$m_{\rm clay}$ (kg kg ⁻¹)	$m_{\rm silt}$ (kg kg ⁻¹)	$m_{\rm gravel}$ (kg kg ⁻¹)	$m_{\rm SOM}$ (kg kg ⁻¹)	$\frac{m_{sand}}{m_{SOM}}$
Sand 2	1.87	1567	0.41	0.548	0.035	0.006	0.001	0.929	0.060	0.010	0	0.001	1327.6
Sand 1	2.19	1567	0.41	0.553	0.029	0.006	0.001	0.939	0.050	0.010	0	0.001	1043.5
Loam 11	1.62	1350	0.49	0.253	0.046	0.208	0.003	0.499	0.090	0.409	0	0.003	199.5
Clay loam 9	1.36	1270	0.52	0.152	0.143	0.181	0.003	0.319	0.299	0.379	0	0.003	118.2
Sandy loam 3	1.68	1333	0.49	0.333	0.060	0.104	0.009	0.664	0.119	0.208	0	0.009	77.2
Loam 4	1.40	1264	0.52	0.189	0.052	0.232	0.005	0.398	0.109	0.488	0	0.005	81.2
Silty clay loam 7	1.34	1267	0.52	0.090	0.128	0.256	0.004	0.189	0.269	0.538	0	0.004	48.5
Silt loam 5	1.38	1272	0.51	0.128	0.104	0.241	0.012	0.267	0.217	0.504	0	0.012	22.4
Silt loam 6	1.47	1255	0.52	0.051	0.089	0.328	0.008	0.109	0.188	0.694	0	0.008	13.0
Silty clay loam 8	1.31	1202	0.52	0.035	0.140	0.263	0.028	0.078	0.310	0.582	0	0.030	2.6

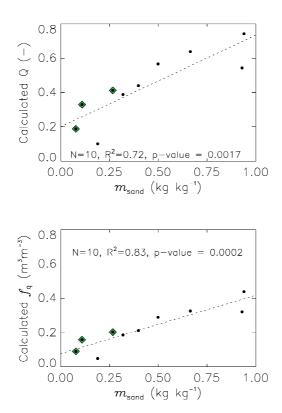


Figure 10 - Gravimetric and volumetric fraction of quartz (top and bottom, respectively) derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) for 10 Chinese soils given by Tarnawski et al. (2009), vs. the gravimetric fraction of sand $m_{\rm sand}$. The three soils for which $m_{\rm sand}/m_{\rm SOM} < 40$ are indicated by green diamonds.

Table 6 – Pedotransfer functions of $f_{\rm q}$ for 7 soils of Lu et al. (2007) with $m_{\rm sand}/m_{\rm SOM} > 40$.

	Regr	ession sco	res			
Predictor of $f_{ m q}$	for 7	Lu soils w	Coefficients			
	$m_{ m san}$	$_{\rm ad}/m_{ m SOM} > 4$				
	r ² RMSD MAE					
	(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 _{sand} *	0.82 (0.005)	0.073	0.054	0.07	0.425	
$m_{ m sand}$	0.82 (0.005)	0.048	0.042	0.04	0.386	
$1-\theta_{\rm sat}-f_{\rm sand}$	0.81 (0.006)	0.050	0.043	0.44	-0.814	

^(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

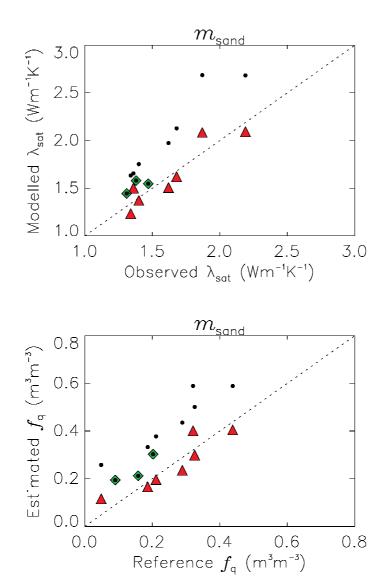


Figure 11 - Estimated $\lambda_{\rm sat}$ and volumetric fraction of quartz $f_{\rm q}$ (top and bottom, respectively) vs. values derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) given by Tarnawski et al. (2009) for 10 Chinese soils, using the gravimetric fraction of sand $m_{\rm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

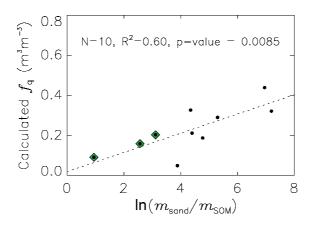


Figure 12 - Volumetric fraction of quartz derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) given by Tarnawski et al. (2009), vs. the logarithm of the $m_{\rm sand}/m_{\rm SOM}$ ratio. The three soils for which $m_{\rm sand}/m_{\rm SOM} < 40$ are indicated by green diamonds.

1.5 [Focus. I believe the pedotransfer function and its evaluation constitute the main contribution of this work. The derivation of soil thermal properties from soil temperature profile, the soil temperature resolution (0.1 C) and its impact on the model applicability can be concise. To me Figure 3 seems dispensable. The Conclusion section also needs revision with a concise description concerning these.]

RESPONSE 1.5

Yes. In the revised version of this work, we will use a slightly more sophisticated q retrieval technique able to cope with soil heterogeneities (see the response to Reviewer 2). The details will be described in a supplement, making the main text more concise.

CHANGES 1.5

Part of the technical developments were moved to Supplements. The evaluation of potential pedotransfer functions is the main focus of the revised version of the paper. A new Section 4.4 addresses the issue of using a single predictor across soil types. It is shown that the gravimetric fraction of sand within soil solids, including gravels and SOM, is a good predictor of the volumetric fraction of quartz when a large variety of soil types is considered.

1.6 [Organization. Section 4.1 is about evaluating impact of gravel and SOM with sensitivity analysis. I suggest it be included/appended following the pedotransfer

functions in the Results section. Indeed authors intended doing so (in Page 740 Line 6 "in Sect 3 a sensitivity analysis of λ sat to SOM and gravel fractions").]

RESPONSE 1.6

We agree. Sect 4.1 will be moved to Sect. 3.

CHANGES 1.6

Sect 4.1 was moved to Sect. 3.3.

1.7 [On Abstract. Authors should do better job in these sections. In Abstract the last three sentences are key results and conclusions of this work and need a great expansion with details; conversely the remaining should be more concise. Please rewrite it and include question, significance, methodology, results, conclusion and this work's impact.]

RESPONSE 1.7

We agree. The Abstract will be rewritten.

CHANGES 1.7

New abstract:

"The information on quartz fraction in soils is usually unavailable but has a major effect on the accuracy of soil thermal conductivity models and on their application in land surface models. This paper investigates the influence of quartz fraction, soil organic matter (SOM) and gravels on soil thermal conductivity. Field observations of soil temperature and water content from 21 weather stations in southern France, along with the information on soil texture and bulk density, are used to estimate soil thermal diffusivity and heat capacity, and then thermal conductivity. The quartz fraction is inversely estimated using an empirical thermal conductivity model. Several pedotransfer functions for estimating quartz content from soil texture information are analysed. It is found that the soil volumetric fraction of quartz (f_0) is systematically better correlated to soil characteristics than the gravimetric fraction of quartz. More than 60 % of the variance of $f_{
m q}$ can be explained using indicators based on the sand fraction. It is shown that SOM and (or) gravels may have a marked impact on thermal conductivity values depending on which predictor of f_q is used. For the grassland soils examined in this study, the ratio of sand to SOM fractions is the best 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 the most robust predictor of f_q when a larger variety of soil types is considered."

1.8 [Page 738 Line 11. "there is no map of q"? Reword to clarify.]

RESPONSE 1.8

We mean that today, q estimates are not given in global digital soil maps. Therefore, land surface modellers need to use a pedotransfer function for q.

1.9 [Page 745 Line 9. How/why is 0.4 chosen/set as cutoff of saturation degree?]

RESPONSE 1.9

In dry conditions, conduction is not the only mechanism for heat exchange in soils, as the convective water vapour flux may become significant (Schelde et al., 1998, Parlange et al. 1998). Also, the K_e functions found in the literature display more variability in dry conditions (see Fig. R1.2). Therefore, this threshold value of $S_d = 0.4$ results from a compromise between the need of limiting the influence of convection, of the shape of the K_e function on the retrieved values of λ_{sat} , and of using as many observations as possible in the retrieval process. For example, if we had taken a threshold of 0.6, we would not have been able to retrieve λ_{sat} for SBR, SVN, LZC, PRD, LGC, BRN, and CBR.

REFERENCES:

Schelde, K., A. Thomsen, T. Heidmann, P. Schjonning and P.-E. Jansson: Diurnal fluctuations of water and heat flows in a bare soil, Water Resour. Res., 34, 11, 2919-2929, 1998.

Parlange, M.B., A.T. Cahill, D.R. Nielsen, J.W. Hopmans, O. Wendroth: Review of heat and water movement in field soils, Soil & Tillage Research, 47, 5-10, 1998.

CHANGES 1.9

Sect. 2.6: "The threshold value of Sd = 0.4 results from a compromise between the need of limiting the influence of convection, of the shape of the Ke function on the retrieved values of λ sat, and of using as many observations as possible in the retrieval process."

1.10 [Page 745 Lines 15-17. I suggest an explicit specifying that the three "contrasting retrieved values of λ sat" are for high, medium and low levels of λ sat values respectively.]

RESPONSE 1.10

Agreed.

CHANGES 1.10

Start of Sect. 3.1: "Figure 3 shows retrieved and modelled 1 values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for contrasting retrieved values of λ_{sat} , from high to low λ_{sat} values (2.80, 1.96, 1.52, and 1.26 Wm-1K-1) at the SBR, MNT, MTM, and PRD stations, respectively."

1.11 [Page 746 Eq 13. I suggest relating this θ satMOD equation to Eq. 12 for quartz pedotransfer function and further to λ sat.]

RESPONSE 1.11

Yes, the use of Eq. (13) in determining a pedotransfer function will be discussed.

CHANGES 1.11

Sect. 3.3: "These results are illustrated in Fig. 8 in the case of the $m_{\rm sand}^*$ pedotransfer function. Figure 8 also shows that using the $\theta_{\rm sat}$ observations instead of $\theta_{\rm satMOD}$ (Eq. (13)) has little impact on $\lambda_{\rm satMOD}$ (Sect. 3.2)."

1.12 [Page 747 Lines 1-4 about Eq 14. I do not see how dMOD is related to λ sat here. I do not see dMOD is mentioned elsewhere. This dMOD is distracting/interruptive to the θ satMOD and can be deleted.]

RESPONSE 1.12

Eq. (14) is equivalent to Eq. (1). The impact of using Eqs. (13)-(14) in the sensitivity study (current Sect. 4.1) will be shown and discussed.

CHANGES 1.12

Sect. 3.3: "These results are illustrated in Fig. 8 in the case of the $m_{\rm sand}^*$ pedotransfer function. Figure 8 also shows that using the $\theta_{\rm sat}$ observations instead of $\theta_{\rm satMOD}$ (Eq. (13)) has little impact on $\lambda_{\rm satMOD}$ (Sect. 3.2)."

1.13 [Page 756 Table 2. The 6 stations with no eligible observations (n = 0), filtered by saturation degree of 0.4, can be simply omitted since they are not informative.]

RESPONSE 1.13

Agreed.

CHANGES 1.13

New Table 2 is as follows:

Table 2 – Thermal properties of 14 grassland soils in southern France: λ_{sat} , f_{q} 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 soils are sorted from the largest to the smallest ratio of m_{sand} to m_{SOM} .

Station	Station full name	λ_{sat} (Wm ⁻¹ K ⁻¹)	RMSD (Wm ⁻¹ K ⁻¹)	n	$f_{\rm q}$ (m ³ m ⁻³)	<i>Q</i> (-)	$\frac{m_{_{sand}}}{m_{_{SOM}}}$
SBR	SABRES	2.80	0.255	6	0.62	0.96	37.2
LGC	LA-GRAND-COMBE	2.07	0.311	20	0.44	0.77	26.6
CBR	CABRIERES-D'AVIGNON	1.92	0.156	20	0.44	0.88	18.4
LZC	LEZIGNAN-CORBIERES	1.71	0.107	20	0.29	0.51	17.3
SVN	SAVENES	1.78	0.163	20	0.34	0.61	15.4
MNT	MONTAUT	1.96	0.058	20	0.42	0.76	13.8
BRN	BARNAS	1.71	0.131	20	0.25	0.40	13.5
SFL	SAINT-FELIX-DE-LAURAGAIS	1.57	0.134	20	0.22	0.37	12.5
MTM	MOUTHOUMET	1.52	0.095	20	0.21	0.35	7.0
URG	URGONS	1.37	0.066	20	0.05	0.10	6.2
LHS	LAHAS	1.57	0.136	20	0.26	0.45	5.3
CDM	CONDOM	1.82	0.086	20	0.26	0.44	5.0
PRG	PEYRUSSE-GRANDE	1.65	0.086	20	0.18	0.32	3.7
PRD	PRADES-LE-LEZ	1.26	0.176	20	0.14	0.28	3.7

1.14 [Page 762 Figure 4 legend. These three stations were chosen as examples to illustrate contrasting levels of λ sat values. I suggest specifying this in legend.]

RESPONSE 1.14

Agreed.

CHANGES 1.14

Start of Sect. 3.1: "Figure 3 shows retrieved and modelled 1 values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for contrasting retrieved values of λ_{sat} , from high to low λ_{sat} values (2.80, 1.96, 1.52, and 1.26 Wm-1K-1) at the SBR, MNT, MTM, and PRD stations, respectively."

1.15 [Page 764 Figure 6. I may have missed, but I do not see the top and middle plots mentioned in the text.]

RESPONSE 1.15

Yes. The Figure is insufficiently discussed in the text. More emphasis will be put on the use of pedotranfer function(s) for quartz in the revised version of this paper.

1.16 [Page 739 Line 15-16. "hydrom-eteorology" should be properly hyphenated as "hydro-meteorology".]

RESPONSE 1.16

Yes. This typo will be corrected.

1.17 [Page 751 Line 16. To be more accurate, change "proposed for quartz" to "proposed for volumetric fraction of quartz".]

RESPONSE 1.17

Agreed.

ESPONSE 1.18	
greed.	
======END ========	

1.18 [Page 760 and page 761. Figure 2 and Figure 3 are misplaced and with wrong

legend; the figures should be swapped if they are to be included.]

Calvet el al. (2015), www.soil-discuss.net/2/737/2015/

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

Response to Reviewer #2 and changes in the revised version of the paper (T. Ren, tsren@cau.edu.cn)

The authors thank Dr. Tusheng Ren (China Agricultural University, Beijing) for his review of the manuscript and for the fruitful comments.

2.1 [This paper investigates the influences of quartz fraction, soil organic matter (SOM) and gravel component on soil thermal conductivity. Field observations of soil temperature and water content from 21 weather stations in southern France, along with the information of soil texture and bulk density, were used to estimated soil thermal diffusivity and heat capacity, and then thermal conductivity. The quartz fraction was inversely estimated with an empirical thermal conductivity model. A pedotransfer function was further proposed for estimating quartz content from soil texture information. The effects of SOM and gravels on thermal conductivity values were also discussed. The information of quartz fraction in a soil is usually unavailable but has a major effect on the accuracy of many thermal conductivity models and their applications in other comprehensive model (e.g., the land-surface models). Therefore, the topic is interesting and has general applications in soil sciences and related areas. However, I have some concerns about the current approach for estimating soil thermal properties and quartz content, the presentation of the results, and the conclusions.]

RESPONSE 2.1

Many thanks for these encouraging comments. We will do our best to account for your remarks in a revised version of the manuscript.

Additional comments

In response to the reviewers' comments, we have revised our approach. The λ retrievals influenced by heterogeneities in soil properties are now sorted out. As a result, we now obtain realistic λ_{sat} values for 14 soils. We improved the assessment of uncertainties on the pedotranfer function for quartz volumetric content:

- a variety of pedotransfer functions is now proposed, not only one
- a confidence interval for the coefficients of pedotransfer functions is given
- the impact of errors on the volumetric heat capacity of soil minerals is assessed
- the data from Lu et al. (2007) are used as an independent benchmark to verify the obtained pedotransfer functions.

In order to clarify the definition of symbols, the volumetric fraction of quartz is now written as " f_q " (instead of "q").

Finally, the Kersten number model of Lu et al. (2005) is now used instead of the Yang et al. (2005) model.

2.2 [First, the method presented in the paper is based mainly on the 1D heat transfer equation and the de Vries (1963) mixed model for soil heat capacity. The authors estimated the apparent soil thermal diffusivity at 10-cm depth from temperature measurements at 5, 10, and 20 cm depths, and calculated soil heat capacity from the information of soil texture, bulk density, and water content at 10 cm. To apply the 1D Fourier heat transfer equation, they assumed that the soil physical properties were uniform and isothermal in the 5-20 cm layer, which was not the case. They stated that "soil properties are relatively homogeneous", but it is difficult to accept this because 1) at least 14 soils had a gravel fraction over 10% (as high as 70% in some soils); 2) there were strong soil moisture and temperature gradients in the 0-20 cm layer; and 3) the existence and spatial distribution of grass roots were ignored. The authors are required to convince the readers that the 0-20 cm soil layer was uniform, and soil temperature and water content measurements at each depth were representative values of the depth.

Otherwise, the soil thermal diffusivity estimates are flawed, and further analysis is invalid.]

RESPONSE 2.2

Yes, we agree. This is a very good point.

We acknowledge that the impact of vertical heterogeneities in λ values has to be properly accounted for in the λ retrieval technique we used. In order to address this issue, we revised our data analysis procedure in order to limit this effect as much as possible. In particular, we used only the soil temperature data presenting a relatively low vertical gradient close to the soil surface, where most differences with deeper layers are found. This refined data sorting increased the λ_{sat} retrieved value for all the stations. A very interesting side effect of the improved procedure was that LHS, SVN, and PRD now present non-zero values of q. On the other hand, the NBN observations are now filtered out as NBN presents very large differences in soil density from one soil depth to another. The new procedure is described below.

The 1D Fourier equation in heterogeneous soil conditions can be written as:

$$C_h \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) \tag{R1}$$

and discretized as:

$$\frac{T_{i}^{n} - T_{i}^{n-1}}{\Delta t} = \frac{1}{C_{hi}} \left[\frac{1}{2} \left(\frac{\lambda_{i+1/2} \gamma_{i+1}^{n} - \lambda_{i-1/2} \gamma_{i}^{n}}{\Delta z_{m}} \right) + \frac{1}{2} \left(\frac{\lambda_{i+1/2} \gamma_{i+1}^{n-1} - \lambda_{i-1/2} \gamma_{i}^{n-1}}{\Delta z_{m}} \right) \right]$$
(R2)

In this study, we assume that the retrieved λ values, at a depth of -0.10m, are representative of a bulk soil layer including the three soil temperature probes used to retrieve the thermal diffusivity, and do not differ much from the interfacial λ values along the bottom and top edges of the considered soil layer ($\lambda_{i+1/2}$ and $\lambda_{i-1/2}$, respectively):

$$\lambda \approx \lambda_{i+1/2} \approx \lambda_{i-1/2}$$
 (R3)

and, at a given time n,

$$\lambda \gamma_{i+1}^n - \lambda \gamma_i^n \approx \lambda_{i+1/2} \gamma_{i+1}^n - \lambda_{i-1/2} \gamma_i^n \tag{R4}.$$

In reality, differences may occur:

$$\Delta \lambda = \lambda_{i+1/2} - \lambda_{i-1/2} \tag{R5}.$$

Considering the temperature gradient ratio R_{TG} at a given time n:

$$R_{TG} = \frac{\gamma_i^n}{\gamma_i^n - \gamma_{i+1}^n} \tag{R6}$$

and combining Eqs. (R4), (R5) and (R6), the retrieved λ can be written as:

$$\lambda \approx \lambda_{i+1/2} - R_{TG} \Delta \lambda$$
 (R7).

Since soil temperature gradients were more pronounced close to the soil surface and since soil density presented smaller values close to the soil surface, the $\Delta\lambda$, R_{TG} , and $R_{TG}\Delta\lambda$ values were ≥ 0 . Since in the soils considered in this study, differences in soil density were much less pronounced at depth than between the -0.05m and -0.10m soil layers, we considered that $\lambda_{i+1/2}$ was closer to the final value to be retrieved, λ^* , than the initial λ retrieval:

$$\lambda^* \approx \lambda + R_{TG} \Delta \lambda$$
 (R8).

Eq. (R8) shows that the target λ^* value is larger than the initial λ retrieval. The relative error on λ^* can be written as $R_{TG}\Delta\lambda/\lambda^*$ (dimensionless). We used $R_{TG}\Delta\lambda/\lambda^*$ as an indicator of the quality of the λ retrieval, with large values of $R_{TG}\Delta\lambda/\lambda^*$ corresponding to erroneous estimates. In the revised data analysis procedure, a subset of 20 λ retrievals per station was used, at most, corresponding to the lowest $R_{TG}\Delta\lambda/\lambda^*$ values, with the condition $R_{TG}\Delta\lambda/\lambda^* < 10\%$. Since the NBN station presented $R_{TG}\Delta\lambda/\lambda^*$ values systematically higher than 10%, the NBN data were excluded from the analysis.

The impact of the refined data selection is illustrated in Fig. R2.1 for the MNT station. For the LHS soil, which presented the highest λ RMSD together with q=0, the new procedure permits obtaining a non-zero value of q (Fig. R2.2).

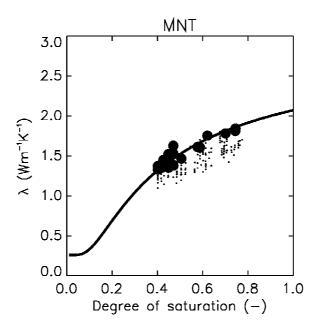


Figure R2.1 - Retrieved and modelled λ values (dots and solid line, respectively) vs. the observed degree of saturation of the soil, at a depth of 0.10 m for the MNT station. The 20 λ retrievals used to fit λ_{sat} are represented by large dots.

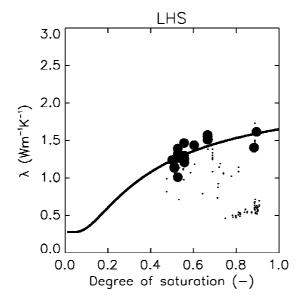


Figure R2.2 - As in Fig. R2.1, except for LHS station.

In practise, the $\Delta\lambda$ term was estimated using top-soil and deep dry density observations (at -0.05m and -0.10m, respectively) and the sensitivity of λ to changes in dry density, $\Delta\lambda/\Delta\rho_d$. The latter was derived numerically using the Eqs. (10)-(13) model, in soil wetness conditions ranging from $S_d = 0.4$ to $S_d = 1$. Since the derivation of $\Delta\lambda/\Delta\rho_d$ depends on the obtained q pedotransfer function (Eq. (12)), $\Delta\lambda/\Delta\rho_d$ values were recalculated with the new pedotransfer function, and a few iterations permitted refining these estimates.

At saturation ($S_d=1$) $\Delta \lambda / \Delta \rho_d$ ranged between $0.64\times 10^{-3}~Wm^2K^{-1}kg^{-1}$ for PRD to $1.24\times 10^{-3}~Wm^2K^{-1}kg^{-1}$ for SBR. At $S_d=0.4$, $\Delta \lambda / \Delta \rho_d$ ranged between $0.46\times 10^{-3}~Wm^2K^{-1}kg^{-1}$ for PRD to $0.81\times 10^{-3}~Wm^2K^{-1}kg^{-1}$ for SBR.

The $\Delta \rho_{\rm d}$ term ranged from 10 kg m⁻³ for CBR to 284 kg m⁻³ for NBN. $R_{\rm TG}$ ranged between 0.5 and 2.4, with a median value of 1.3.

CHANGES 2.2

The data selection method described above was included in a Supplement, together with Fig. S2.1. It is mentioned that the NBN, PZN, BRZ, and MJN observations are completely filtered out using the condition $R_{\rm TG}\Delta\lambda/\lambda^* < 10\%$.

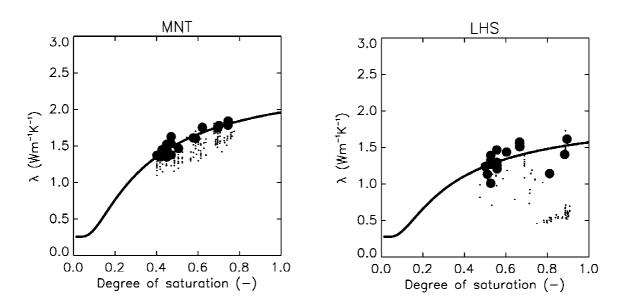


Figure S2.1 - Retrieved and modelled λ values (dots and solid line, respectively) vs. the observed degree of saturation of the soil, at a depth of 0.10 m for the MNT and LHS stations. The 20 λ retrievals used to fit $\lambda_{\rm sat}$ are represented by large dots.

2.3 [Second, the de Vries (1963) mixing model was applied to estimate soil volumetric heat capacity. To do so, a fixed value of 2.0 MJ m-3 K-1 was used for soil solids. The authors should give justification to use a constant value for the 21 soils with different

textures. Tarara and Ham (1997) used a value of 1.92 MJ m-3 K-1. A soil-specific value may be better for estimating the volumetric heat capacity of soil solids.]

RESPONSE 2.3

Yes, soil-specific values for the volumetric heat capacity of soil minerals (C_{hmin}) may be more appropriate than using a constant standard value. However, we were not able to find such values in the literature and we did not measure this quantity.

We investigated the sensitivity of our results to these uncertainties, considering the following minimum and maximum C_{hmin} values: $C_{\text{hmin}} = 1.8 \text{ J m}^{-3} \text{ K}^{-1}$ and $C_{\text{hmin}} = 2.2 \text{ J m}^{-3} \text{ K}^{-1}$. The impact of C_{hmin} on the retrieved values of λ_{sat} and q is presented in Figs. R2.3 and R2.4, respectively. The impact of C_{hmin} on the q pedotransfer function will be published in the final version of this work.

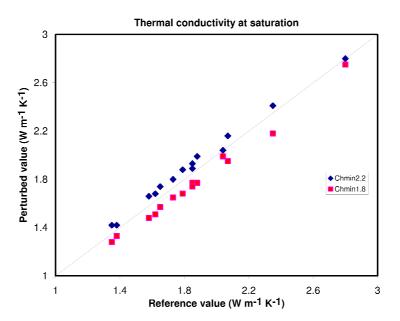


Figure R2.3 - Impact on the retrieved λ_{sat} of using values of $C_{\text{hmin}} = 1.8 \text{ J m}^{-3} \text{ K}^{-1}$ and $C_{\text{hmin}} = 2.2 \text{ J m}^{-3} \text{ K}^{-1}$ instead of $C_{\text{hmin}} = 2.0 \text{ J m}^{-3} \text{ K}^{-1}$.

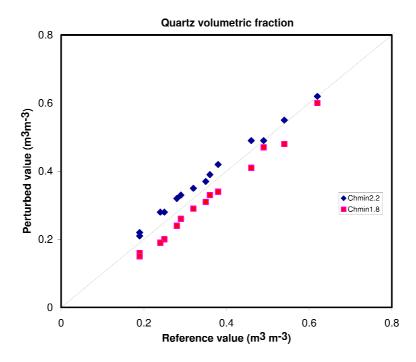


Figure R2.4 - As in Fig. R2.3, except for volumetric fraction of quartz.

CHANGES 2.3 (Sect. 4.1)

"In this study, the de Vries (1963) mixing model is applied to estimate soil volumetric heat capacity, and a fixed value of 2.0 MJ m⁻³ K⁻¹ is used for soil minerals (Eq. (6)). Soil-specific values for $C_{\rm hmin}$ may be more appropriate than using a constant standard value. For example, Tarara and Ham (1997) used a value of 1.92 MJ m⁻³ K⁻¹. 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 $C_{\rm hmin}$ values: $C_{\rm hmin} = 1.92$ MJ m⁻³ K⁻¹ and $C_{\rm hmin} = 2.08$ MJ m⁻³ K⁻¹. The impact of $C_{\rm hmin}$ on the retrieved values of $\lambda_{\rm sat}$ and $f_{\rm q}$ is presented in Fig. 9. On average, a change of + (-) 0.08 MJ m⁻³ K⁻¹ in $C_{\rm hmin}$ triggers a change in $\lambda_{\rm sat}$ and $f_{\rm q}$ of + 1.7 % (-1.8 %) and + 4.8 % (-7.0 %), respectively."

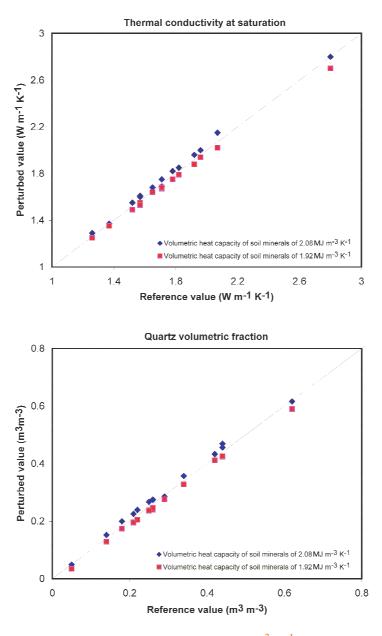


Figure 9 - Impact of using values of $C_{\rm hmin} = 1.92$ MJ m⁻³ K⁻¹ and $C_{\rm hmin} = 2.08$ MJ m⁻³ K⁻¹ instead of $C_{\rm hmin} = 2.0$ MJ m⁻³ K⁻¹ on (top) the retrieved $\lambda_{\rm sat}$, (bottom) the volumetric fraction of quartz.

REFERENCES:

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.

Tarara, J.M., and J.M. Ham: Measuring soil water content in the laboratory and field with dual-probe heat-capacity sensors, Agron. J., 89, 535–542, 1997.

2.4 [In addition, what were the volumetric fractions of grass roots in the 0-20 cm soil layer? Does the heat capacity of grass roots have a significant influence on the bulk soil heat capacity?]

RESPONSE 2.4

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⁻² 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 $\leq 0.0005 \text{ kg kg}^{-1}$, i.e. less than 4% of the lowest m_{SOM} values observed in this study (0.013 kg kg⁻¹) 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 λ retrievals.

CHANGES 2.4

New Sect. 4.1: "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⁻² 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 ≤ 0.0005 kg kg⁻¹, i.e. less than 4% of the lowest $m_{\rm SOM}$ values observed in this study (0.013 kg kg⁻¹) or less than 5% of $f_{\rm SOM}$ values. We checked that increasing $f_{\rm SOM}$ values by 5% has negligible impact on heat capacity and on the λ retrievals".

REFERENCE:

Calvet, J.-C., Bessemoulin, P., Noilhan, J., Berne, C., Braud, I., Courault, D., Fritz, N., Gonzalez-Sosa, E., Goutorbe, J.-P., Haverkamp, R., Jaubert, G., Kergoat, L., Lachaud, G., Laurent, J.-P., Mordelet, P., Olioso, A., Péris, P., Roujean, J.-L., Thony, J.-L., Tosca,

C., Vauclin, M., Vignes, D.: MUREX: a land-surface field experiment to study the annual cycle of the energy and water budgets, Ann. Geophys., 17, 838-854, 1999.

2.5 [Third, no independent data or measurements were used to evaluate the estimates of soil thermal conductivity and quartz fraction. In Table 2, for example, the estimated thermal conductivity values for saturated soils ranged from 0.52 to 2.79 W m-1 K-1 for 15 soils, all were much lower than the published results of Lu et al. (2007) and Tarnawski et al. (2011). The authors may need to verify the results by compare the model estimates against thermal conductivity measurements with the line-source probe or the heat pulse technique.]

RESPONSE 2.5

It must be noted that in many studies (e.g. Lu et al., 2007) λ_{sat} estimates are derived from reassembled sieved soil samples excluding the gravels, while our data concern undisturbed soils.

In our revised analysis, we found λ_{sat} values ranging between 1.26 Wm⁻¹K⁻¹ and 2.80 Wm⁻¹K⁻¹. These values are consistent with λ_{sat} values reported by other authors. Tarnawski et al. (2011) gave λ_{sat} values ranging between 2.5 Wm⁻¹K⁻¹ and 3.5 Wm⁻¹K⁻¹ for standard sands. Lu et al. (2007) gave λ_{sat} values ranging between 1.33 Wm⁻¹K⁻¹ and 2.2 Wm⁻¹K⁻¹.

CHANGES 2.5

New Sect. 4.3 (Applicability of the new λ_{sat} model to other soil types) uses the Lu et al. (2007) data as an independent benchmark.

2.6 [Finally, I do not think the empirical equations (13) and (14), and related results and discussion, are related to and helpful for the purpose of this paper.]

RESPONSE 2.6

The empirical Eq. (13) for θ_{sat} is used for the end-to-end simulation for the sensitivity study of Table 3, as such an equation has to be used in land surface models. Eq. (14) is equivalent to

Eq. (1). The impact of using Eq. (13) in the sensitivity study (current Sect. 4.1) will be shown and discussed. Note that we found and corrected a bug in the program we developed to perform this sensitivity analysis. In the revised manuscript, the sensitivity study will be performed with and without using this equation, and for several plausible pedotransfer functions.

CHANGES 2.6

Sect. 3.2: "Modelled values of $\lambda_{\rm sat}$ ($\lambda_{\rm satMOD}$) can be derived from $f_{\rm qMOD}$ using Eq. (10) together with $\theta_{\rm sat}$ observations. The $\lambda_{\rm satMOD}$ r^2 , RMSD, and mean bias scores are given in Table 5. Again, the best scores are obtained using the $m_{\rm sand}/m_{\rm SOM}$ predictor of $f_{\rm q}$, with r^2 , RMSD, and mean bias values of 0.86, 0.14 Wm⁻¹K⁻¹, and +0.01 Wm⁻¹K⁻¹, respectively (Fig. 7)."

Sect. 3.3: "Figure 8 shows that using the θ_{sat} observations instead of θ_{satMOD} (Eqs. (13)) has little impact on λ_{satMOD} (Sect. 3.2)."

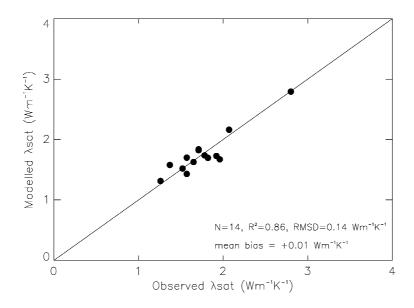


Figure 7 – $\lambda_{\text{sat}MOD}$ values derived from the m_{sand} / m_{SOM} pedotransfer function for the volumetric quartz fractions, using observed θ_{sat} values, vs. λ_{sat} retrievals.

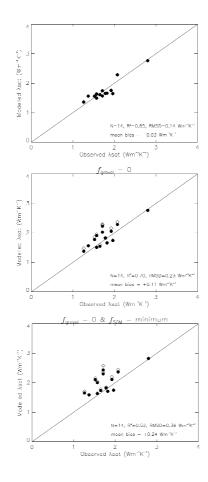


Figure 8 – λ_{satMOD} values derived from the m_{sand}^* pedotransfer function for the volumetric quartz fractions, using or not θ_{satMOD} (Eq. (13)) (dark dots and opened diamonds, respectively), vs. λ_{sat} retrievals: (top) full model, (middle) $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$, (bottom) $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$ and $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$.

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

Model configuration	Predictor of $f_{ m q}$	r^2	RMSD (Wm ⁻¹ K ⁻¹)	Mean bias (Wm ⁻¹ K ⁻¹)
Model using θ_{sat} observations	$m_{ m sand} / m_{ m SOM} \ m_{ m sand}^* \ m_{ m sand} \ 1 - heta_{ m sat} - f_{ m sand}$	0.86 0.83 0.81 0.82	0.14 0.15 0.16 0.16	+0.01 -0.01 -0.03 -0.03
Full model using θ_{satMOD} (Eqs. (13))	$m_{ m sand} / m_{ m SOM} \ m_{ m sand} * \ m_{ m sand}$	0.85 0.85 0.84	0.14 0.14 0.15	+0.03 -0.03 -0.03

	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.82	0.16	-0.02
same with:	$m_{\mathrm{sand}} / m_{\mathrm{SOM}}$	0.57	0.35	+0.20
$f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$	$m_{ m sand}*$	0.83	0.15	+0.00
	$m_{ m sand}$	0.81	0.16	-0.02
	$1-\theta_{\mathrm{sat}}-f_{\mathrm{sand}}$	0.83	0.15	-0.02
same with:	$m_{\rm sand} / m_{\rm SOM}$	0.87	0.19	-0.12
$f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$	$m_{ m sand}*$	0.70	0.23	+0.11
	$m_{ m sand}$	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
$f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$	$m_{ m sand}*$	0.52	0.36	+0.24
and $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$	$m_{ m sand}$	0.59	0.29	+0.16
y g.u.o.	$1 - \theta_{\rm sat} - f_{\rm sand}$	0.70	0.25	+0.16

^(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

2.7 [The current title does not fully represent the content of this paper. The title talks about the effects of gravels and organic matter on soil thermal conductivity values. In the text, on the other hand, the authors spent a lot effort on discussing the influences of quartz content on soil thermal conductivity. The title also addresses the grassland soils, but the detailed information about grass cover and roots was missing.]

RESPONSE 2.7

Yes, in the revised version of the manuscript, the effects of gravels and organic matter on soil thermal conductivity values will be included in the result section. More information of vegetation characteristics will be given.

CHANGES 2.7

Title: "gravels and organic matter" was replaced by "quartz".

Section 3: Sect. 4.1 was moved to Sect. 3.3.

New Sect. 4.1: "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⁻² 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 $\leq 0.0005 \text{ kg kg}^{-1}$, i.e. less than 4% of the lowest m_{SOM} values observed in this study (0.013 kg kg⁻¹) 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 λ retrievals".

2.8 [Page 739 Line 7-8: The authors stated that soil thermal conductivity was hard to obtain directly and in situ. This is not true today. Recent advances in line-source probe and heat pulse method have made it easy to monitor soil thermal conductivity in the field (e.g., Bristow, K.L., G.J. Kluitenberg, and R. Horton. 1994. Measurement of soil thermal properties with a dual-probe heat-pulse method. Soil Sci. Soc. Am. J. 58:1288–129; Zhang, X., J. Heitman, R. Horton and T. Ren. 2014. Measuring near-surface soil thermal properties with the heat-pulse method: correction of ambient temperature and soil—air interface effects. Soil Sci. Soc. Am. J. 78:1575–1583. The authors may also include the reference of Bristow (1998) who investigated the influences of quartz fraction on soil thermal conductivity.]

RESPONSE 2.8

Yes, this sentence will be rephrased. Note however that such measurements are currently not made in operational meteorological networks. 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 (e.g. https://ismn.geo.tuwien.ac.at/).

CHANGES 2.8

Introduction:

"The construction and the verification of the λ models is not easy as λ 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 method have made it easier to monitor soil thermal conductivity in the field (Bristow et al., 1994; Zhang et al., 2014), such measurements are currently not made in operational meteorological networks."

"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 implement (Schönenberger et al., 2012). This has a major effect on the accuracy of thermal conductivity models and their applications (Bristow, 1998)."

2.9 [Page 740 Line 21: Fig. 2 should be cited as Fig. 3 here. Page 741 Line 17: 'Figure 3' should be 'Figure 2'.]

RESPONSE 2.9

Yes. This typo will be corrected.

2.10 [Page 740 Line 23-26: How were gravel and SOM contents determined? Grass roots may also influence soil thermal conductivity and heat capacity in the shallow soil layers, but were ignored in the paper. Please give supporting evidence about this. In addition, what depth was bulk density measured? Did soil bulk density differ with depth?]

RESPONSE 2.10

Soil texture, gravel and SOM fractions were measured by an independent laboratory we contracted (INRA-Arras) from samples we collected in situ.

We checked that grass roots should not significantly influence our results (see RESPONSE 2.4). One cannot exclude large root density values very close to the soil surface during the plant growth period, but the new data sorting procedure we implemented limits these soil heterogoneity effects (see RESPONSE 2.2).

Bulk density was measured at all depths (-0.05 m, -0.10 m, -0.20 m) using unperturbed oven-dried soil samples collected using metal cylinders of known volume. Most differences were observed from -0.05 m to -0.10 m, as soil density is lower close to the surface. The largest difference was observed for NBN (-284 kg m⁻³ at -0.05 m with respect to -0.10 m, or -18%). For the 14 stations now presenting successful q retrieval, -0.05 m density relative differences with respect to density at -0.10 m range from $\pm 3\%$ or less (MNT, SFL, LGC, CBR, LHS, SVN, PRD) to about -13% (SBR, BRN, PRG), and from -7% to -9% for CDM, LZC, MTM, and URG.

CHANGES 2.10

See Supplement 1 (Table S1.1) and Supplement 2.

2.11 [Sect. 2.5: The estimated thermal conductivity values were used to retrieve quartz content data using the empirical thermal conductivity models. Leong et al. (2009) tried to use the Lu et al. (2007) model to inversely estimate quartz content in soil samples. In this work, the authors used the Yang et al. (2005) model. Please explain why the Yang et al. (2005) model was used, and how the quartz content estimates from the two models may differ.]

RESPONSE 2.11

Yes, in the first version of this work, we used the Kersten number calculation used by Yang et al. (2005). Figure R2.5 shows the resulting K_e value, together the K_e value obtained using the Lu et al. (2007) model for fine and coarse soils. It can be seen that most differences between these models occur for S_d values < 0.4. Since we only use λ retrievals for S_d values > 0.4, the impact of the uncertainties in the determination of K_e is limited. However, using Lu et al. (2007) instead of Yang et al. (2005) tends to produce smaller values of λ_{sat} and q retrievals, as shown by Figs. R2.6 and R2.7. The impact of the Kersten number calculation will be discussed in the final version of this work.

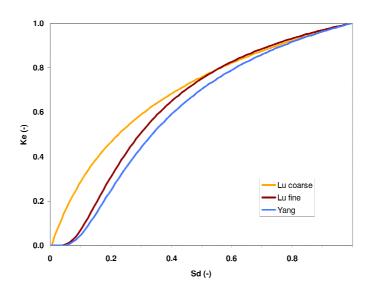


Figure R2.5 - Kersten number vs. degree of saturation as modelled by Lu et al. (2007) for coarse and fine soils, and as modelled by Yang et al. (2005).

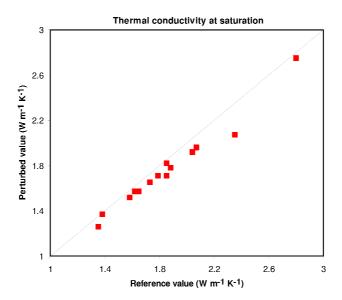


Figure R2.6 - λ_{sat} retrievals using the Kersten number as modelled by Lu et al. (2007) vs. those using the Kersten number as modelled by Yang et al. (2005).

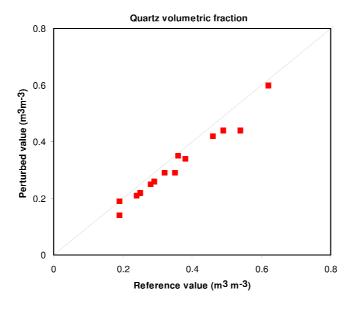


Figure R2.7 - As in Fig. R2.6, except for *q* retrievals.

CHANGES 2.11 (Sect. 2.5)

"In this study, the formula recommended by Lu et al. (2007) is used:

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

with $\alpha = 0.96$ for $Mn_{\rm sand} \ge 0.4$ kg kg⁻¹, $\alpha = 0.27$ for $Mn_{\rm sand} < 0.4$ kg kg⁻¹, and $S_d = \theta/\theta_{sat}$

 $Mn_{\rm sand}$ represents the sand mass fraction of fine earth minerals (values are given in Supplement 1).

Following Peters-Lidard et al. (1998), λ_{other} is taken as 2.0 Wm⁻¹K⁻¹ for soils with Mn_{sand} $> 0.2 \text{ kg kg}^{-1}$, and 3.0 Wm⁻¹K⁻¹ otherwise. In this study, $Mn_{\text{sand}} > 0.2 \text{ kg kg}^{-1}$ for all soils except for URG, PRG, and CDM."

2.12 [Sect. 2.6: More in-depth explanations are required to explain the calculation of quartz content.]

RESPONSE 2.12

Yes, we will publish a Supplement to the final version of the paper explaining the various calculation steps.

CHANGES 2.12 (Sect. 2.6)

"Only λ observations for S_d values higher than 0.4 are used because in dry conditions:, (1) conduction is not the only mechanism for heat exchange in soils, as the convective water vapour flux may become significant (Schelde et al., 1998, Parlange et al. 1998), (2) the K_e functions found in the literature display more variability, (3) the λ_{sat} retrievals are more sensitive to uncertainties in λ observations. The threshold value of $S_d = 0.4$ results from a compromise between the need of limiting the influence of convection, of the shape of the K_e function on the retrieved values of λ_{sat} , and of using as many observations as possible in the retrieval process."

(9).

2.13 [Sect. 3.2: I am not sure how useful to develop the pedotransfer functions for estimating quartz content. It is apparent that all errors in the measurement (e.g., temperature, water content, bulk density, and gravel fraction) and calculations (thermal diffusivity and heat capacity) have been included in the results of quartz content. In addition, I had a hard time to figure out how quartz content was related to the fraction of soil organic matter (Eq. [12]).]

RESPONSE 2.13

In the revised version of the manuscript, we will improve the description and the assessment of the uncertainties affecting the obtained pedotransfer function(s).

CHANGES 2.13

We improved the assessment of uncertainties on the pedotranfer function for quartz volumetric content:

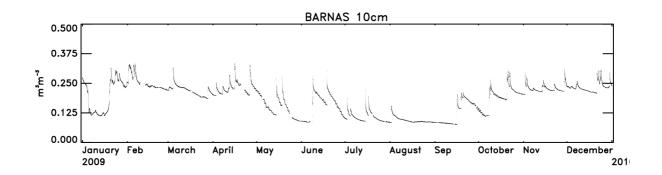
- a variety of pedotransfer functions is now proposed, not only one
- a confidence interval for the coefficients of pedotransfer functions is given
- the impact of errors on the volumetric heat capacity of soil minerals is assessed
- the data from Lu et al. (2007) are used as an independent benchmark to verify the obtained pedotransfer functions.

2.14 [Sect. 4.2: The authors suggested that the very low values of quartz content might be caused by (1) the natural heterogeneity of soil properties, (2) the living root biomass, and (3) stones that were not accounted for in the gravel fraction. All these factors lead to inaccurate estimates of soil thermal diffusivity and heat capacity. Therefore, I wonder if it is correct to include all the 21 stations in this work. On those soils with high fractions of gravel (and stones) and grass roots, it is impossible to obtain representative temperature and water content data at each depth, and it is inappropriate to apply the 1D heat transfer equation to estimate soil thermal diffusivity.]

RESPONSE 2.14

The difficulties we had can be explained by heterogeneities in soil properties, soil density in particular. An enhanced procedure was implemented in order to mitigate this effect (see RESPONSE 2.2). LHS, SVN, and PRD now present non-zero values of q and the NBN

observations are filtered out. We had no difficulty in measuring soil temperature and soil moisture, including at the BRN soil presenting the largest fraction of gravel (see Fig. R2.8). Note that the sensors we use are designed to work in such difficult conditions. The ThetaProbe and PT100 sensors have very strong rods, 0.06 m and 0.10 m long, respectively.



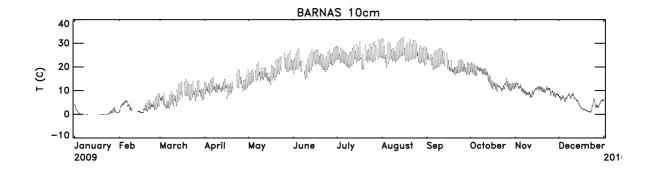


Figure R2.8 - Soil temperature and soil moisture measured in 2009 at the BRN station at a depth of -0.10m

CHANGES 2.14 (Supplement 1)

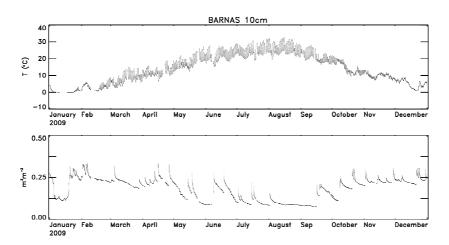


Figure S1.2 - Soil temperature (top) and volumetric soil moisture (bottom) measured in 2009 at the Barnas station (BRN) at a depth of –0.10m.

2.15 [Most symbols in this paper are not properly defined.]

RESPONSE 2.15

We tried to use symbols used in other works. It will be made clear that in this study, q (f_{SOM}) represents the volumetric fraction of quartz (SOM) within the whole soil volume, while in many studies, it represents the volumetric fraction of quartz (SOM) within the volume of soil solids.

CHANGES 2.15 (Sect. 2.5, Eq. (11))

In order to clarify the definition of symbols, the volumetric fraction of quartz is now written as " f_q " (instead of "q"):

$$f_q = Q \times (1 - \theta_{sat})$$

with Q representing the fraction of quartz within soil solids.

2.16 [Table 1: The soil texture should be mentioned together with the particle size distribution.]

RESPONSE 2.16

A new table will be added, listing the particle size distribution observations.

CHANGES 2.15

Supplement 1, Table S1.1.

2.17 [Figure 2 and 3 do not match with their captions.]

RESPONSE 2.17

Yes. This typo will be corrected.

2.18 [Figure 4: How were the solid lines obtained? For the SBR site, why a large variation in thermal conductivity was observed in a narrow range of degree of saturation? How come a gravel soil (the PRD site) had very low thermal conductivity in the degree of saturation range of 0.4-0.5 range?]

RESPONSE 2.18

For several soils (SBR, SVN, LZC, PRD, LGC, BRN, and CBR), no λ retrieval or very few λ retrievals were obtained for $S_d > 0.6$. Since we did not use the data for Sd < 0.4, a narrow range of S_d is used for these soils. In the revised analysis (see RESPONSE 2.2), the lowest λ retrieval values are not considered as they result from heterogeneities in soil density.

CHANGES 2.18

Sect. 2.6: "The threshold value of Sd=0.4 results from a compromise between the need of limiting the influence of convection, of the shape of the Ke function on the retrieved values of λ sat, and of using as many observations as possible in the retrieval process."

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

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12 January 2016<mark>26 March 2015</mark>

Abstract

The information on quartz fraction in soils is usually unavailable but has a major effect on the accuracy of soil thermal conductivity models and on their application in land surface models. This paper investigates the influence of quartz fraction, soil organic matter (SOM) and gravels on soil thermal conductivity. Field observations of soil temperature and water content from 21 weather stations in southern France, along with the information on soil texture and bulk density, are used to estimate soil thermal diffusivity and heat capacity, and then thermal conductivity. The quartz fraction is inversely estimated using an empirical thermal conductivity model. Several pedotransfer functions for estimating quartz content from soil texture information are analysed. It is found that the soil volumetric fraction of quartz (f_g) is systematically better correlated to soil characteristics than the gravimetric fraction of quartz. More than 60 % of the variance of f_g can be explained using indicators based on the sand fraction. It is shown that SOM and (or) gravels may have a marked impact on thermal conductivity values depending on which predictor of f_g is used. For the grassland soils examined in this study, the ratio of sand to SOM fractions is the best predictor of f_g . 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_{α} when a larger variety of soil types is considered. 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_b) 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.

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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

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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 (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 earth, only. Today, f_0 estimates are not given in global digital soil maps and it is often assumed 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 (λ) , in Jm⁻³K⁻¹ and Wm⁻¹K⁻¹, respectively. Provided the volumetric fractions of moisture, minerals and organic matter are known, Ch 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; Tarnawski 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; 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 (Bristow et al., 1994; Zhang et al., 2014), such measurements are currently not made in operational meteorological networks. 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 information on quartz fraction in a soil fraction of quartz is usually unavailable 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). This has a major effect on the accuracy of thermal conductivity models and their applications (Bristow, 1998). 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 gravimetric fraction of quartz (40) is equal to the volumetric gravimetric fraction of sand within mineral fine earth (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 subhourly 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 information on soil moisture, soil texture, soil gravel content, soil organic matter, and bulk density, λ values are derived from soil thermal diffusivity and heat capacity. The response of λ to soil moisture is investigated and the feasibility of modelling the λ value at saturation ($\lambda_{\rm sat}$)

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with or without using SOM and gravel fraction observations is assessed using an empirical thermal conductivity model based on Lu et al. (2007). The volumetric fraction of quartz, f_{q^-} , q^- values are is retrieved by reverse modelling together with Q_7 . Pedotransfer functions are further proposed for estimating quartz content from soil texture information.

The field data and the method to retrieve λ values are presented in Sect. 2. The λ and f_{qq} 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. Technical details are given in Supplements.

2. Data and methods

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119 2.1. The SMOSMANIA data

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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 Meteo-France, upgraded with four soil moisture probes at four depths: 0.05 m, 0.10 m, 0.20 m, 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. 2see Supplement 1). At the same time, Fig. 2 shows that soil texture does not vary much with depth (from 0.05 m 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 7×10⁻⁴ m³). 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

140 soil moisture and soil temperature probes consisted of Thetaprobe ML2X and PT100 sensors, 141 respectively. 142 The ThetaProbe sensors provide a voltage signal in units of V. In order to convert the voltage signal into volumetric soil moisture content (m³ m⁻³), site-specific calibration curves were 143 144 developed using in situ gravimetric soil samples for all stations, and for all depths (Albergel et 145 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 146 147 of exponential curves in the previous version of the data set. 148 The soil temperature observations are recorded with a resolution of 0.1 °C. 149 The observations from the 48 soil moisture probes and from the 48 temperature probes are 150 automatically recorded every 12 minutes. The data are available to the research community 151 through the International Soil Moisture Network web site (https://ismn.geo.tuwien.ac.at/). Figure 23 shows soil temperature time series at the Saint-Félix-de-Lauragais (SFL) station on 23 152 February 2015. The impact of recording temperature with a resolution of 0.1 °C is clearly visible 153 154 at all depths as this causes a levelling of the curves. 155 In this study, sub-hourly measurements of soil temperature and soil moisture at a depth of 0.10 m 156 are used, together with soil temperature measurements at 0.05 m and 0.20 m, from 1 January 157 2008 to 28-30 February September 2015. 158 159

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 (θ_{sat}), is derived from the bulk dry density ρ_{d} , together with soil texture and soil organic matter observations as:
- $\theta_{sat} = 1 \rho_d \left[\frac{m_{sand} + m_{clay} + m_{silt} + m_{gravel}}{\rho_{\min}} + \frac{m_{SOM}}{\rho_{SOM}} \right]$

166 or

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

- 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 $\rho_{\rm d}$
- observations to ρ_x , the density of each soil component x. Values of $\rho_{SOM} = 1300 \text{ kg m}^{-3}$ and $\rho_{min} =$
- 171 2660 kg m⁻³ are used for soil organic matter, and soil minerals, respectively.
- 173174 2.3. Retrieval of soil thermal diffusivity
- The soil thermal diffusivity (D_h) is expressed in m²s⁻¹ and is defined as:

$$D_h = \frac{\lambda}{C_h} \tag{2}$$

- 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 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:

$$_{181} C_h \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) (3).$$

- 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:

$$_{184} \quad \frac{\partial T}{\partial t} = D_h \frac{\partial^2 T}{\partial z^2} \tag{4}$$

- 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
- 188 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,
- 191 $z_2 = -0.10$ 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
- 193 Crank-Nicholson scheme. When three soil depths are considered, z_{i-1} , z_i , z_{i+1} , the change in soil
- 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
- 195 written as:

$$_{196} \quad \frac{T_{i}^{n} - T_{i}^{n-1}}{\Delta t} = D_{hi} \left[\frac{1}{2} \left(\frac{\gamma_{i+1}^{n} - \gamma_{i}^{n}}{\Delta z_{m}} \right) + \frac{1}{2} \left(\frac{\gamma_{i+1}^{n-1} - \gamma_{i}^{n-1}}{\Delta z_{m}} \right) \right] \quad \text{with}$$

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

- 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.
- It is important to ensure that D_h retrievals are related to diffusion processes only and not to the
- transport of heat by water infiltration or evaporation (Parlange et al., 1998; Schelde et al., 1998).

- Therefore, only situations for which changes in soil moisture at all depths do not exceed 0.001
- 203 m^3m^{-3} within the Δt time lag are considered.

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205 2.4. From soil diffusivity to soil thermal conductivity

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

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

- where θ and f_{min} represent the volumetric soil moisture and the volumetric fraction of soil
- 213 <u>minerals, respectively.</u> and vV alues 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 for C_{hwater} , C_{hmin} , C_{hSOM} , respectively.
- The λ values at 0.10 m are then derived from the D_h and C_h estimates (Eq. (2)).

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217 2.5. Soil thermal conductivity model

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

$$\lambda_{dry} = 0.51 - 0.56 \times \theta_{sat} \qquad \text{(in Wm-1K-1)}$$
 (7)

- When soil pores are gradually filled with water, λ tends to increase towards a maximum value at
- saturation (λ_{sat}). Between dry and saturation conditions, λ 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, θ , i.e. to the
- degree of saturation (S_d). In this study, the formula recommended by $\frac{\text{Yang-Lu}}{\text{Lu}}$ et al. ($\frac{20052007}{\text{Lu}}$)
- is used:

$$K_e = \exp\{\alpha \left(1 - S_d^{(\alpha - 1.33)}\right)\} K_e = \exp(k_T \left(1 - 1/S_d\right)),$$

229 with $\alpha = 0.96$ for $Mn_{\text{sand}} \ge 0.4$ kg kg⁻¹, $\alpha = 0.27$ for $Mn_{\text{sand}} < 0.4$ kg kg⁻¹, and

with
$$k_T = 0.36$$
 and $S_d = \theta/\theta_{sat}$

231 ____(9).

- 232 <u>Mn_{sand} represents the sand mass fraction of mineral fine earth (values are given in Supplement 1).</u>
- Following Peters-Lidard et al. (1998), λ_{other} is taken as 2.0 Wm⁻¹K⁻¹ for soils with $Mn_{sand} > 0.2$
- kg kg⁻¹, and 3.0 Wm⁻¹K⁻¹ otherwise. In this study $Mn_{\text{sand}} > 0.2$ kg kg⁻¹ for all soils, except for
- 235 URG, PRG, and CDM.
- The geometric mean equation for λ_{sat} proposed by Johansen (1975) for the mineral components
- of the soil can be generalized to include the SOM thermal conductivity (Chen et al., 2012) as:

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

- (10)
- where q- f_q is the volumetric fraction of quartz, and $\lambda_q = 7.7 \text{ Wm}^{-1}\text{K}^{-1}$, $\lambda_{other} = 2.0 \text{ Wm}^{-1}\text{K}^{-1}$, λ_{water}
- 242 = 0.594 Wm⁻¹K⁻¹, $\lambda_{SOM} = 0.25$ Wm⁻¹K⁻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:

$$f_{other} = 1 - f_q - \theta_{sat} - f_{SOM}$$

 $\underset{\text{246}}{\text{with}} f_q = Q \times (1 - \theta_{sat})$ (11)

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2.6. Reverse modelling

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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 Wm⁻¹K⁻¹ to 4 Wm⁻¹K⁻¹, with a resolution of 0.01 $Wm^{-1}K^{-1}$. The λ_{sat} retrieval corresponds to the λ simulation presenting the lowest root mean square difference (RMSD) value with respect to the λ observations. Only λ observations for S_d values higher than 0.4 are used, because in dry conditions: (1) conduction is not the only mechanism for heat exchange in soils, as the convective water vapour flux may become significant (Schelde et al., 1998, Parlange et al. 1998), (2) the K_e functions found in the <u>literature display more variability, (3)</u> the λ_{sat} retrievals are <u>very more</u> sensitive to uncertainties in λ observations—obtained in dry conditions.. The threshold value of $S_d = 0.4$ results from a compromise between the need of limiting the influence of convection, of the shape of the K_e function on the retrieved values of λ_{sat} , and of using as many observations as possible in the retrieval process. Moreover, the data filtering technique to limit the impact of soil heterogeneities, described in Supplement 2, is used to select valid λ observations. Finally, the $\underline{f_{qq}}$ 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

269 270	2.7. Scores
271	Pedotransfer functions for quartz and λ_{sat} are evaluated using the following scores:
272	• the Pearson correlation coefficient (r) , and the squared correlation coefficient (r^2) is used
273	to assess the fraction of explained variance,
274	• the RMSD,
275	• the Mean Absolute Error (MAE), i.e. the mean of absolute differences,
276	• the mean bias, i.e. the mean of differences.
277	In order to test the predictive and generalization power of the pedotransfer regression equations, a
278	simple bootstrapping resampling technique is used. It consists in calculating a new estimate of $f_{\rm q}$
279	for each soil using the pedotransfer function obtained without using this specific soil. Gathering
280	these new f_q estimates, one can calculate new scores with respect to the retrieved f_q values. Also,
281	this method provides a range of possible values of the coefficients of the pedotransfer function
282	and permits assessing the influence of a given f_q retrieval on the final result.
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283 3. Results 284 285 3.1. λ_{sat} and \underline{f}_{qq} retrievals 286 287 288 Retrievals of $\lambda_{\rm sat}$ and $f_{\rm q}$ could be obtained for 14 soils. Figure 34 shows retrieved and modelled λ 289 290 values vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for contrasting retrieved values of λ_{sat} , from high to low λ_{sat} values (2.8079, 1.9645, 1.52, and 1.260.70 291 Wm⁻¹K⁻¹) at the SBR, MNT, MTM, and PRD stations, respectively. 292 All the obtained λ_{sat} and f_{op} retrievals are listed in Table 2, together with the λ RMSD values and 293 294 the number of available selected λ observations. For six-three stations soils (CRD, PZN, MZN, 295 and VLV, MJN, and BRZ), the reverse modelling technique described in Sect. 2.6 cannot could 296 <u>not</u> be <u>implemented applied</u> as not enough λ observations could be obtained for S_d values higher 297 than 0.4. For four soils (NBN, PZN, BRZ, and MJN), all the λ retrievals were filtered out as the 298 obtained values were influenced by heterogeneities in soil density (see Supplement 2). For the 299 other 145 stations soils, λ_{sat} and f_{qq} retrievals a were obtained using a subset of 20 λ retrievals per 300 soil, at most, corresponding to the soil temperature data presenting the lowest vertical gradient 301 close to the soil surface (Supplement 2). 62 to 1939 λ observations. For the five stations (LHS, 302 SVN, NBN, and PRD) presenting the lowest λ_{sat} retrievals, ranging between 0.52 and 1.11 Wm⁻¹K⁻¹, null values of q are obtained. The λ model (Eqs. (7) (11)) is fully operative, with non-303 304 null values of q, for eleven stations: SBR, URG, PRG, CDM, MNT, SFL, MTM, LZC, LGC, BRN, CBR. 305 306

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3.2 A pPedotransfer functions for quartz

The f_qq retrievals can be used to assess the possibility to estimate f_qq 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_{sand} or m_{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_{gravel} and f_{gravel} + f_{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 λ_{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:

- 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, RMSD= $0.09 \text{ m}^3 \text{m}^{-3}$). However, a better result is found considering the
- 324 sum of the fractions of the other soil particles, and the modelled q values can be derived from the
- 325 following pedotransfer function:

$$326 f_{qMOD} = a_0 + a_1 \times P$$

327 and
$$f_{qMOD} \le 1 - \theta_{sat} - f_{SOM}$$
 or $q_{MOD} = 0.70 - 1.075 \times (1 - \theta_{sat} - f_{sand})$

$$328 (12)$$

- 329 where P represents the predictor of $f_q(r^2 = 0.78$, F test p value = 0.0003, RMSD=0.07 m³m⁻³).
- 330 The values of q_{MOD} vs. q are shown in Fig. 5.

331 The a_0 and a_1 coefficients are given in Table 3 for four pedotransfer functions based on the best predictors of f_0 . The pedotranfer functions are illustrated in Fig. 6. The scores are displayed in 332 333 Table 4. The bootstrapping indicates that the SBR sandy soil has the largest individual impact on 334 the obtained regression coefficients. This is why the scores without SBR are also presented in 335 Table 4. For the $m_{\rm sand}$ predictor, a r^2 value of 0.56 is obtained without SBR, against a value of 0.67 when 336 337 all the 14 soils are considered. An alternative to this $m_{\rm sand}$ pedotransfer function consists in considering only $m_{\rm sand}$ values smaller than 0.6 kg kg⁻¹ in the regression, thus excluding the SBR 338 339 soil. The corresponding predictor is called $m_{\rm sand}^*$. In this configuration, the sensitivity of $f_{\rm q}$ to <u>m_{sand}</u> is much increased (with $a_1 = 0.944$, against $a_1 = 0.572$ with SBR). For SBR, f_q is 340 overestimated by the m_{sand} * equation but this is corrected by the f_{qMOD} limitation of Eq. (12), and 341 in the end a better r^2 score is obtained when the 14 soils are considered ($r^2 = 0.74$). 342 Values of r^2 larger than 0.7 are obtained for two predictors of f_0 : $m_{\text{sand}}/m_{\text{SOM}}$ and m_{sand} *. A value 343 of $r^2 = 0.65$ is obtained for $1 - \theta_{\text{sat}} - f_{\text{sand}}$ (the fraction of soil solids other than sand). The 344 $m_{\rm sand}/m_{\rm SOM}$ predictor presents the best r^2 and RMSD scores in all the configurations (regression, 345 346 bootstrap, and regression without SBR). Another characteristic of the m_{sand}/m_{SOM} pedotransfer 347 function is that the confidence interval for the a_0 and a_1 coefficients derived from bootstrapping is 348 narrower than for the other pedotransfer functions (Table 3), indicating a more robust relationship 349 of f_0 with $m_{\text{sand}}/m_{\text{SOM}}$ than with other predictors. 350 Modelled values of λ_{sat} ($\lambda_{\text{sat}MOD}$) can be derived from $\underline{f_{\text{qMOD}}q_{\text{MOD}}}$ using Eq. (10) together with θ_{sat} observations. and tThe λ_{satMOD} following r^2 , RMSD, and mean bias scores are obtained for 351 $\lambda_{\text{sat}MOD}$, with respect to the λ_{sat} retrievals: 0.87, 0.15 Wm⁻¹K⁻¹, and 0.01 Wm⁻¹K⁻¹, respectively 352 (Table 3) given in Table 5. Again, the best scores are obtained using the $m_{\text{sand}}/m_{\text{SOM}}$ predictor of 353

- 354 f_{g} , with r^2 , RMSD, and mean bias values of 0.86, 0.14 Wm⁻¹K⁻¹, and +0.01 Wm⁻¹K⁻¹, respectively
- 355 (Fig. 7).
- 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
- 358 relationship between θ_{satMOD} , m_{clay} , m_{silt} , and m_{SOM} :

359
$$\theta_{satMOD} = 0.456 - 0.0735 \frac{m_{clay}}{m_{silt}} + 2.238 m_{SOM}$$
 (13)

- 360 ($r^2 = 0.48$, F-test p-value = 0.0027, RMSD=0.036 m³m⁻³).
- Volumetric fractions of soil components need to be consistent with θ_{satMOD} and can be calculated
- using the modelled bulk density values, derived from θ_{satMOD} as: using Eq. (1).

363
$$\underline{\rho_{dMOD}} = \frac{1 - \theta_{satMOD}}{\underline{m_{sand} + m_{clay} + m_{silt} + m_{gravel}} + \underline{m_{SOM}}}$$

$$\underline{\rho_{min}} + \underline{m_{SOM}}$$

$$\underline{\rho_{SOM}}$$
(14).

- Equations (1010) to (134) constitute an empirical end-to-end model of λ_{sat} . Table 3-5 shows that
- using θ_{satMOD} (Eqs. (13)_(14)) instead of the θ_{sat} observations has little impact on the λ_{satMOD}
- 366 scores.

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368 4. Discussion 369 370 3.34.1. Impact of gravels and SOM on $\frac{q}{q}$ and λ_{sat} 371 372 Gravels and SOM are often neglected in soil thermal conductivity models used in LSMs. 373 Moreover, it is often assumed that q is equal to f_{sand} . The Eqs. (10)-(134) empirical model 374 obtained in Sect. 3.2 permits the assessment of the impact of $\frac{1}{q}$, f_{gravel} and f_{SOM} on λ_{sat} . Table $\frac{3-5}{2}$ 375 shows the impact on $\lambda_{\text{sat}MOD}$ scores of imposing <u>a</u> null values to of f_{gravel} and <u>a small value of f_{SOM} </u> 376 to all the soils. and of assuming $q = f_{\text{sand}}$. The combination of these assumptions is evaluated, 377 also. Imposing $f_{SOM} = 0.013 \text{ m}^3\text{m}^{-3}$ (the smallest f_{SOM} value, observed for CBR) has a limited impact 378 379 on the scores, except for the $m_{\rm sand}/m_{\rm SOM}$ pedotransfer function. In this case, $\lambda_{\rm sat}$ is overestimated 380 by $+0.20 \text{ Wm}^{-1}\text{K}^{-1}$, 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 381 (overestimation) of $\lambda_{\rm sat}$ for the $m_{\rm sand}/m_{\rm SOM}$ ($m_{\rm sand}$ *) pedotransfer function, by $-0.12~{\rm Wm}^{-1}{\rm K}^{-1}$ 382 $(+0.11 \text{ Wm}^{-1}\text{K}^{-1}).$ 383 384 On the other hand, iIt appears that combining these assumptions has a marked impact on all the <u>pedotransfer functions.</u> Nneglecting gravels $(f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3})$ and imposing $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$ 385 386 has a major impact on λ_{sat} : the modelled λ_{sat} is overestimated by all the pedotransfer functions (with a mean bias of ranging from +0.165 Wm⁻¹K⁻¹ to +0.24 Wm⁻¹K⁻¹) and $r^2 = 0.65$ is markedly 387 smaller, especially for the $m_{\rm sand}$ and $m_{\rm sand}$ * pedotransfer functions. while the full model is 388 virtually unbiased and presents a r^2 value of 0.87. These results are illustrated in Fig. 8 in the case 389

of the $m_{\rm sand}$ * pedotransfer function. Figure 8 also shows that using the $\theta_{\rm sat}$ observations instead of

391	$\underline{\theta_{\text{satMOD}}}$ (Eq. (13)) has little impact on λ_{satMOD} (Sect. 3.2) but tends to enhance the impact of
392	neglecting gravels. A similar result is found with the m_{sand} pedotransfer function (not shown).
393	Neglecting SOM also triggers an overestimation of λ_{sat} (+0.12 Wm ⁻¹ K ⁻¹) but has no impact on r^2 .
394	On the other hand, although neglecting SOM while accounting for gravels has no impact on r^2 ,
395	neglecting SOM tends to amplify the detrimental impact of neglecting gravels: $r^2 = 0.51$ and the
396	mean bias is equal to +0.41 Wm ⁻¹ K ⁻¹ . Assuming $q = f_{\text{sand}}$ tends to trigger an underestimation of
397	λ_{sat} (−0.22 Wm ⁻¹ K ⁻¹), and to compensate for the bias caused by neglecting SOM. Combining Eq.
398	(12) and Eq. (1), it appears that Eq. (12) boils down to $q = 1.075 \times f_{\text{sand}}$ for θ_{sat} values close to
399	$0.35 \text{ m}^3\text{m}^3$. For higher θ_{sat} values, q tends to be higher than $1.075 \times f_{\text{sand}}$. Since θ_{sat} is higher than
400	$0.35 \text{ m}^3\text{m}^{-3}$ at all the sites (Table 1), the $q = f_{\text{sand}}$ assumption tends to underestimate q and,
401	subsequently, λ_{sat} .
402	Table 3 shows that in the configuration representative of most soil thermal conductivity models
403	currently used in LSMs (i.e. neglecting gravels and SOM while assuming $q = f_{\text{sand}}$), only 61 % of
404	the λ_{sat} variance is explained by the model ($r^2 = 0.61$), and λ_{sat} is markedly overestimated (the
405	mean bias is equal to +0.24 Wm ⁻¹ K ⁻¹). The impact of this model configuration is illustrated in
406	Fig. 6 (bottom), together with the impact of $q = f_{\text{sand}}$ alone.
407	Finally, the correlation of the retrieved values of q with the volumetric fraction of solids is
408	analysed in Table 4. Using f_{sand} as a predictor of q gives a r^2 -value of 0.66, against 0.78 for Eq.
409	(12). Gravels and silt have the largest impact on r^2 ($r^2 = 0.12$ and $r^2 = 0.38$, respectively).
410	
411	4. Discussion
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 $4.\underline{1}2$. Sources of uncertainties in heat capacity estimates Null values of q

414 Null values of q are obtained for four stations: LHS, SVN, NBN, and PRD (Table 2 and Fig. 4). 415 They correspond to the lowest values of the λ_{sat} retrievals, ranging from 0.52 to 1.11 Wm⁻¹K⁻¹. 416 417 Such values can be encountered for organic soils (e.g. Chen et al., 2012) of for volcanic ash soils 418 (Tarnawski et al., 2009) but are surprising for the soil types considered in this study. On the other hand, it must be noted that Eq. (12) predicts very low values of q for $f_{\text{elay}} + f_{\text{silt}} + f_{\text{silt}}$ 419 $f_{\text{eravel}} + f_{\text{SOM}}$ close to 0.65 m³m⁻³. All the retrieved null values of q are obtained below this 420 threshold (Fig. 4), from 0.43 to 0.54 m³m⁻³. Therefore, a possible marked underestimation of 421 either f_{elay} , f_{silt} , f_{gravel} , or f_{SOM} may explain these discrepancies, or the overestimation of f_{sand} or θ_{sat} . 422 423 In this study, the de Vries (1963) mixing model is applied to estimate soil volumetric heat capacity, and a fixed value of 2.0×10⁶ Jm⁻³K⁻¹ is used for soil minerals (Eq. (6)). Soil-specific 424 values for C_{hmin} may be more appropriate than using a constant standard value. For example, 425 Tarara and Ham (1997) used a value of 1.92×10⁶ Jm⁻³K⁻¹. However, we did not measure this 426 427 quantity and we were not able to find such values in the literature. 428 We investigated the sensitivity of our results to these uncertainties, considering the following minimum and maximum C_{hmin} values: $C_{\text{hmin}} = 1.92 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1}$ and $C_{\text{hmin}} = 2.08 \times 10^6 \text{ J m}^{-3}$ 429 K^{-1} . The impact of changes in C_{hmin} on the retrieved values of λ_{sat} and f_{q} is presented in Fig. 9. On 430 average, a change of + (-) 0.08×10^6 J m⁻³ K⁻¹ in C_{hmin} triggers a change in λ_{sat} and f_{q} of + 1.7 % 431 432 (-1.8 %) and +4.8 % (-7.0 %), respectively. The impact of changes in C_{hmin} on the regression coefficients of the pedotransfer functions is 433 434 presented in Table 3 (last column). The impact is very small, except for the a_1 coefficient of the

 $\underline{m_{\text{sand}}}^*$ pedotransfer function. However, even in this case, the impact of C_{hmin} on the a_1 coefficient

is much lower than the confidence interval given by the bootstrapping, indicating that the

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137	relatively small number of soils considered in this study (as in other studies, e.g. Lu et al. (2007))
138	is a larger source of uncertainty.
139	Moreover, uUncertainties in the se f_{clay} , f_{silt} , f_{gravel} , or f_{SOM} fractions may be caused by (1) the
140	natural heterogeneity of soil properties, (2) the living root biomass, (3) stones that <u>are may not be</u>
141	accounted for in the gravel fraction.
142	In particular, during the installation of the probes, it was observed that stones are present at the
143	foursome stations. Stones are not evenly distributed in the soil, and it is not possible to
144	investigate whether the soil area where the temperature probes were inserted contains stones as it
145	must be left unperturbed.
146	The grasslands considered in this study are not intensively managed. They consist of set-aside
147	fields cut once or twice a year. Calvet et al. (1999) gave an estimate of 0.160 kg m ⁻² for the root
148	dry matter content of such soils for a site in southwestern France, with most roots contained in
149	the 0.25m top soil layer. This represents a gravimetric fraction of organic matter smaller than
150	$0.0005 \text{ kg kg}^{-1}$, i.e. less than 4% of the lowest m_{SOM} values observed in this study $(0.013 \text{ kg kg}^{-1})$
151	or less than 5% of f_{SOM} values. We checked that increasing f_{SOM} values by 5% has negligible
152	impact on heat capacity and on the λ retrievals.
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156	4.3. Applicability of the new λ_{sat} model to other soil types
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158	The λ_{sat} values found in this study are consistent with values reported by other authors. In this
159	study, λ_{sat} values ranging between 1.26 Wm ⁻¹ K ⁻¹ and 2.80 Wm ⁻¹ K ⁻¹ are found (Table 2).

Tarnawski et al. (2011) gave λ_{sat} values ranging between 2.5 Wm⁻¹K⁻¹ and 3.5 Wm⁻¹K⁻¹ for 460 standard sands. Lu et al. (2007) gave λ_{sat} values ranging between 1.33 Wm⁻¹K⁻¹ and 2.2 461 462 $Wm^{-1}K^{-1}$. A key component of the $\lambda_{\rm sat}$ model is the pedotransfer function for quartz (Eq. (12)). The $f_{\rm q}$ 463 464 pedotranfer functions proposed in this study are based on basic soil characteristics. The current global soil digital maps provide information about SOM, gravels and bulk density (Nachtergaele 465 466 et al., 2012). Therefore, using Eq. (1) and Eqs. (6)-(12) at large scale is possible, and porosity can 467 be derived from Eq. (1).—On the other hand, the suggested f_0 pedotranfer functions are obtained for temperate grassland soils containing a rather large amount of organic matter, and are valid for 468 469 <u>m_{sand}/m_{SOM}</u> ratio values lower than 40 (Table 2). These equations should be evaluated for other 470 regions. In particular, hematite has to be considered together with quartz for tropical soils. 471 Moreover, while the pedotransfer function we get for θ_{sat} (Eq. (13)) is valid for the specific sites 472 considered in this study and is used to conduct the sensitivity study of Sect. 3.3, Eq. (13) cannot 473 be used to predict porosity in other regions. 474 A key component of the $\lambda_{\rm sat}$ model proposed in this study is the pedotransfer function for quartz 475 476 (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 477 478 sandy soils and in such conditions, one should ensure that $q \le f_{\text{sand}}$. 479 While the pedotransfer function we get for θ_{sat} (Eq. (13)) is valid for the specific sites considered 480 in this study and is used to conduct the sensitivity study of Sect. 4.1, Eq. (13) cannot be used to 481 predict porosity in other regions.

482	In order to assess the applicability of the pedotransfer function for quartz obtained in this study,
483	we used the independent data from Lu et al. (2007) and Tarnawski et al. (2009), for ten Chinese
484	soils (see Supplement 3 and Table S3.1). These soils consist of reassembled sieved soil samples
485	and contain no gravel, while our data concern undisturbed soils. Moreover, most of these soils
486	contain very little organic matter and the $m_{\rm Sand}/m_{\rm SOM}$ ratio can be much larger that the $m_{\rm Sand}/m_{\rm SOM}$
487	values measured at our grassland sites. For the 14 French soils used to determine pedotransfer
488	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
489	et al. (2007) present such low values of $m_{\rm Sand}/m_{\rm SOM}$. The other seven soils of Lu et al. (2007)
490	present $m_{\text{sand}}/m_{\text{SOM}}$ values ranging from 48 to 1328 (see Table S3.1).
491	We used λ_{sat} experimental values derived from Table 3 in Tarnawski et al. (2009) to calculate Q
492	and f_q for the ten Lu et al. (2007) soils. Figure 10 shows the statistical relationship between these
493	quantities and m_{sand} . Very good correlations of Q and f_{q} with m_{sand} are observed, with r^2 values of
494	0.72 and 0.83 , respectively. This is consistent with our finding that f_q is systematically better
495	correlated to soil characteristics than Q (Sect. 3.2).
496	The pedotransfer functions derived from French soils tend to overestimate f_q for the Lu el al.
497	(2007) soils, especially for the seven soils presenting $m_{\text{sand}}/m_{\text{SOM}}$ values larger than 40. Note that
498	Lu et al. (2007) obtained a similar result for coarse-textured soils with their model, which
499	assumed $Q = m_{\text{sand}}$. For the three other soils, presenting $m_{\text{sand}}/m_{\text{SOM}}$ values smaller than 40, f_{q}
500	MAE values are given in Table 4. The best MAE score (0.071 m ³ m ⁻³) is obtained for the m_{sand} *
501	$\underline{predictor}\ of\ f_{\underline{q}}.$
502	These results are illustrated by Fig. 11 for the $m_{\rm sand}$ predictor of $f_{\rm q}$. Figure 11 also shows the $f_{\rm q}$
503	and λ_{sat} estimates obtained using specific coefficients in Eq. (12), based on the seven Lu et al.
504	(2007) soils presenting $m_{\text{sand}}/m_{\text{SOM}}$ values larger than 40. These coefficients are given together

505 with the scores in Table 6. Table 6 also present these values for other predictors of f_q . It appears 506 that $m_{\rm sand}$ gives the best scores. The contrasting coefficient values between Table 6 and Table 3 507 (Chinese and French soils, respectively) illustrate the variability of the coefficients of 508 pedotransfer functions from one soil category to another, and the $m_{\rm sand}/m_{\rm SOM}$ ratio seems to be a 509 good indicator of the validity of a given pedotransfer function. On the other hand, the $m_{\rm sand}/m_{\rm SOM}$ ratio is not a good predictor of $f_{\rm q}$ for the Lu et al. (2007) soils 510 presenting $m_{\rm sand}/m_{\rm SOM}$ values larger than 40, and r^2 presents a small value of 0.40 (Table 6). This 511 512 can be explained by the very large range of $m_{\rm sand}/m_{\rm SOM}$ values for these soils (see Table S3.1). 513 Using $ln(m_{sand}/m_{SOM})$ instead of m_{sand}/m_{SOM} is a way to obtain a predictor linearly correlated to f_q . 514 This is shown by Fig. 12 for the ten Lu et al. (2007) soils: the correlation is increased to a large extent $(r^2 = 0.60)$. 515 516 517 4.4. Can m_{sand} -based f_0 pedotransfer functions be used across soil types? 518 Given the results presented in Tables 3, 4, and 6, it can be concluded that m_{sand} is the best 519 predictor of f_q across mineral soil types. The $m_{\rm sand}/m_{\rm SOM}$ predictor is relevant for the mineral soils 520 containing the largest amount of organic matter. 521 The results presented in this study suggest that the $m_{\rm sand}/m_{\rm SOM}$ ratio can be used to differentiate 522 temperate grassland soils containing a rather large amount of organic matter (3.7 $< m_{\rm sand}/m_{\rm SOM} <$ 523 40) from soils containing less organic matter ($m_{\text{sand}}/m_{\text{SOM}} > 40$). The m_{sand} predictor can be used 524 in both cases, with the following a_0 and a_1 coefficient values in Eq. (12): 0.15 and 0.572 for 525 $m_{\rm sand}/m_{\rm SOM}$ ranging between 3.7 and 40 (Table 3), and 0.04 and 0.386 for $m_{\rm sand}/m_{\rm SOM} > 40$ (Table 526 6), respectively.

527 <u>Although the $m_{\text{Sand}}/m_{\text{SOM}}$ predictor gives the best r^2 scores for the 14 grassland soils considered in 528 this study, it seems more difficult to apply this predictor to other soils, as shown by the high</u>

529 MAE score (MAE = $0.135 \text{ m}^3\text{m}^{-3}$) for the corresponding Lu et al. (2007) soils in Table 4.

Moreover, the scores are very sensitive to errors in the estimation of m_{SOM} as shown by Table 5.

Although the m_{sand} * predictor gives slightly better scores than m_{sand} (Table 4), the a_1 coefficient in

more sensitive to errors in C_{hmin} (Table 3), and the bootstrapping reveals large uncertainties in a_0

533 and a_1 values.

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535 4.<u>5</u>4. Prospects for using soil temperature profiles

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537 Using standard soil moisture and soil temperature observations is a way to investigate soil

538 thermal properties over a large variety of soils, as the access to such data is facilitated by online

539 <u>databases (Dorigo et al., 2013).</u>

A key-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 %.

Since T_i is recorded with a resolution of

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

546 the retrieved D_h values are affected by uncertainties and the relative uncertainty of D_h can be

547 estimated as:

$$\frac{\left|\partial D_{hi}\right|}{\left|D_{hi}\right|} = \Delta T_{i} \times \left[\frac{1}{\left|T_{i}^{n} - T_{i}^{n-1}\right|} + \frac{\Delta z_{i+1}^{-1} + \Delta z_{i}^{-1}}{\left|\gamma_{i+1}^{n} - \gamma_{i}^{n}\right| + \left|\gamma_{i+1}^{n-1} - \gamma_{i}^{n-1}\right|} \right]$$
(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 0900 LST and 1400 LST),

and at dusk to a lesser extent, between 1700 LST and 0000 LST. In this study, we have imposed

the following conditions for using the obtained D_h retrievals:

$$|T_i^n - T_i^{n-1}| > 0.8 \, {}^{\circ}C_{\rightarrow} |\gamma_{i+1}^n - \gamma_i^n| > 30Km^{-1}_{\rightarrow} |\gamma_{i+1}^{n-1} - \gamma_i^{n-1}| > 30$$

555 According to Eq. (7), this ensures that

$$\begin{array}{c|c}
 & \partial D_{hi} \\
\hline
D_{hi} & 18\%
\end{array}$$
(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. (S4.317). 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 °C only. More precision in the λ estimates would permit investigating other processes of heat transfer in the soil such as those related to water transport (Rutten, 2015).

5. Conclusions

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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 48minute 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 $^{\circ}$ 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 145 stations. The Lu et al. (2007)A empirical elassic 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, aA number of pedotransfer functions is proposed for volumetric fraction of quartz, for the considered region in France. For the grassland soils examined in this study, the ratio of sand to SOM fractions is the best predictor of f_q . A sensitivity study shows that gravels have a major impact on λ_{sat} and that omitting gravels and the SOM information has a major impact on λ_{sat} tends to enhance this impact. Eventually, an error propagation analysis and a comparison with independent $\lambda_{\rm sat}$ data from Lu et al. (2007) show that the gravimetric fraction of sand within soil solids, including gravels and SOM, is a good predictor of the volumetric fraction of quartz when a larger variety of soil types is considered. 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 1 – Soil characteristics at 10 cm for the 21 stations of the SMOSMANIA network. Porosity values are derived from Eq. (1). Solid fraction values higher than 0.3 are in bold. The stations are listed from West to East (from top to bottom). ρ_d , θ_{sat} , f, and m, stand for soil bulk density, porosity, volumetric fractions, and gravimetric fractions, respectively.

Station Soil	ρ _d (kg m ⁻³)	θ_{sat} (m ³ m ⁻³)	f_{sand} (m ³ m ⁻³	f_{clay}) (m ³ m ⁻³)	f_{silt} (m ³ m ⁻³)	f_{gravel}) (m ³ m ⁻³)	f_{SOM} (m ³ m ⁻³)	<i>m</i> _{sand}) (kg kg ⁻¹)	m _{clay} (kg kg ⁻¹)	m _{silt}) (kg kg ⁻¹)	m _{gravel} (kg kg ⁻¹)	m _{SOM} (kg kg)
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: λ_{sat} , f_{q} 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 soils are sorted from the largest to the smallest ratio of m_{sand} to m_{SOM} .

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

 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	$\lambda_{\text{sat}} = (Wm^{-1}K^{-1})$	$q \cdot (m^3 m^{-3})$	RMSD (Wm ⁻¹ 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	MOUTHOUMET	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

<u>Table 3</u> — 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	* ²	RMSD (Wm ⁻¹ K ⁻¹)	Mean bias (Wm ⁻¹ 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)
$- same with: f_{SOM} = 0$	-0.87 (0.00)	0.23 (1.18)	+0.12 (+0.78)
same with: $f_{SOM} = 0$ and $q = f_{sand}$	-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)
$- same with: f_{gravel} = 0$	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)
$- same with: f_{gravel} = 0 \text{ and } f_{SOM} = 0$	0.51 (0.01)	0.56 (1.34)	+0.41 (+1.01)

Predictor of q	* ²	RMSD (m ³ m ⁻³)
$\frac{f_{\text{elay}} + f_{\text{silt}} + f_{\text{gravel}} + f_{\text{SOM}}}{f_{\text{elay}} + f_{\text{silt}} + f_{\text{gravel}}}$ $\frac{f_{\text{silt}} + f_{\text{gravel}} + f_{\text{SOM}}}{f_{\text{sand}}}$ $\frac{f_{\text{clay}}}{f_{\text{elay}} + f_{\text{silt}}} + f_{\text{SOM}}$	0.78 0.78 0.67 0.66 0.38 0.12	0.07 0.07 0.09 0.09 0.12 0.14

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 729 Table 3 - Coefficients of four pedotransfer functions of f_q for 14 soils of this study, together
 730 with indicators of the coefficient uncertainty, derived by bootstrapping and by perturbing the

volumetric heat capacity of soil minerals (C_{hmin}). The best predictor is in bold.

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	Coefficients	s for 14 soils	Confide	nce interval	Impact of a change of		
Predictor of f_q			<u>from bo</u>	otstrapping	$\pm 0.08 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1} \text{ in}$		
					<u>(</u>	<u>-hmin</u>	
	<u>a</u> ₀	<u>a</u> 1	<u>a</u> ₀	<u>a</u> ₁	<u>a</u> 0	<u>a</u> ₁	
m _{sand} /m _{SOM}	0.12	0.0134	[0.10,0.14]	[0.012,0.014]	[0.11,0.13]	[0.013,0.013]	
<u>m_{sand}*</u>	<u>0.08</u>	0.944	[0.00,0.11]	[0.85,1.40]	[0.07,0.09]	[0.919,0.966]	
<u>m</u> _{sand}	<u>0.15</u>	0.572	[0.08,0.17]	[0.54,0.94]	[0.14,0.17]	[0.55,0.56]	
$1 - \theta_{\rm sat} - f_{\rm sand}$	<u>0.73</u>	<u>-1.020</u>	[0.71,0.89]	[-1.38, -0.99]	[0.70,0.73]	[-1.00, -0.99]	

732 (*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

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

	Regression scores			Bootstrap scores			Scores without SBR		
Predictor of f_q							(and N	MAE for 3	<u>Lu soils)</u>
	<u>r</u> ²	RMSD	MAE	<u>r</u> ²	RMSD	MAE	<u>r</u> 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
<u> </u>	<u>0.77</u>	<u>0.007</u>	<u>0.033</u>	0.72	0.074	0.002	0.02	<u>0.070</u>	<u>(0.135)</u>
<u>m_{sand}*</u>	<u>0.74</u>	<u>0.072</u>	0.052	<u>0.67</u>	<u>0.126</u>	<u>0.100</u>	<u>0.56</u>	0.075	<u>0.056</u> (0.071)
<u>m_{sand}</u>	<u>0.67</u>	<u>0.081</u>	0.060	<u>0.56</u>	0.121	0.084	<u>0.56</u>	0.075	<u>0.056</u> (0.086)
$1 - \theta_{\mathrm{sat}} - f_{\mathrm{sand}}$	<u>0.65</u>	0.084	0.064	<u>0.56</u>	0.102	0.079	<u>0.45</u>	0.084	<u>0.061</u> (0.158)

^(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

Table 5 – Ability of the Eqs. (10)-(13) empirical model to estimate λ_{sat} values for 14 soils and 144 impact of changes in gravel and SOM volumetric content: $f_{\text{gravel}} = 0 \text{ m}^3 \text{m}^{-3}$ and $f_{\text{SOM}} = 0.013$ might will be mallest f_{SOM} value, observed for CBR). r^2 values smaller than 0.60, RMSD values higher than 0.20 Wm⁻¹K⁻¹, and mean bias values higher (smaller) than +0.10 (-0.10) are in bold.

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

(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

750 <u>Table 6 - Pedotransfer functions of fq for 7 soils of Lu et al. (2007) with m_{sand}/m_{SOM} > 40. The
 751 <u>best predictor and the best scores are in bold.</u>
</u>

	Regr	ession sco			
Predictor of f_q	<u>for 7</u>	Lu soils w	<u>Coefficients</u>		
	<u>m</u> san	$\frac{1}{100}$ $\frac{1}{100}$ $\frac{1}{100}$	<u> 10</u>		
	<u>r</u> ²	<u>RMSD</u>	MAE		
	<u>(p-value)</u>	(m^3m^{-3})	(m^3m^{-3})	<u>a</u> 0	<u>a</u> 1
$m_{\rm sand}/m_{\rm SOM}$	0.40 (0.13)	0.089	0.075	0.20	0.000148
<u>m_{sand}*</u>	0.82 (0.005)	0.073	0.054	<u>0.07</u>	0.425
<u>M_{Sand}</u>	0.82 (0.005)	0.048	0.042	0.04	0.386
$1 - \theta_{\text{sat}} - f_{\text{sand}}$	0.81 (0.006)	0.050	0.043	<u>0.44</u>	<u>-0.814</u>

(*) only m_{sand} values smaller than 0.6 kg kg⁻¹ are used in the regression

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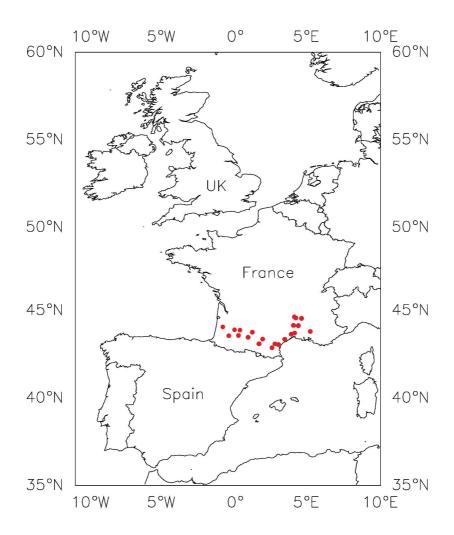


Fig. 1 – Location of the 21 SMOSMANIA stations in southern France.

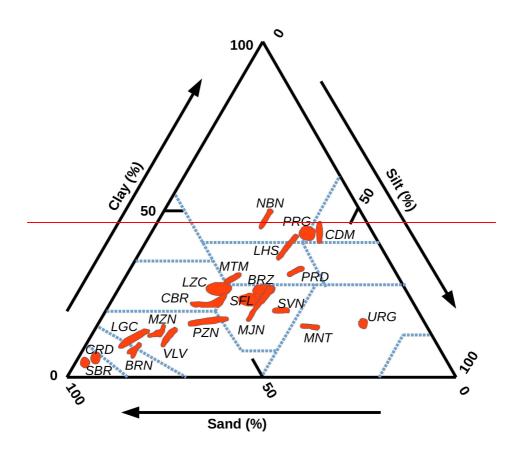


Fig. 2—Soil characteristics of the 21 SMOSMANIA stations at a depth of 10cm: mineral fine earth gravimetric fractions of clay, silt and sand. For a given station, the red mark covers the fraction values measured at 0.05, 0.10 and 0.20 m. Full station names are given in Table 2. The dashed blue lines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

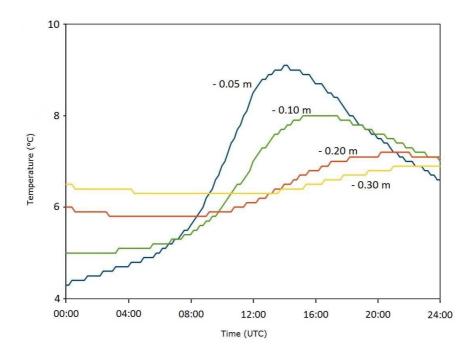
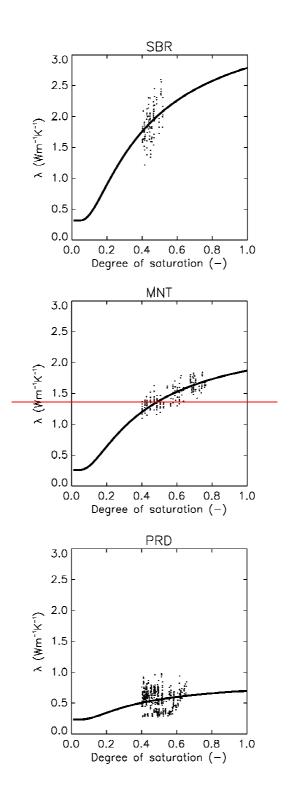


Fig. 23 – Soil temperature measured at the Saint-Félix-de-Lauragais (SFL) station on 23 | February 2015, at depths of 0.05, 0.10, 0.20, and 0.30 m. Levelling is due to the low resolution of the temperature records (0.1°C).



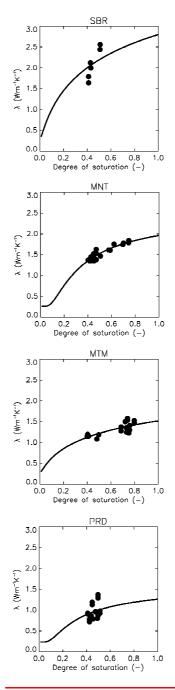


Fig. 34 – Retrieved λ values (dark dots) vs. the observed degree of saturation of the soil, at a depth of 0.10 m, for (from top to bottom) Sabres (SBR), Montaut (MNT), Mouthoumet (MTM), and Prades-le-Lez (PRD), together with simulated λ values from dry to wet conditions (dark lines).

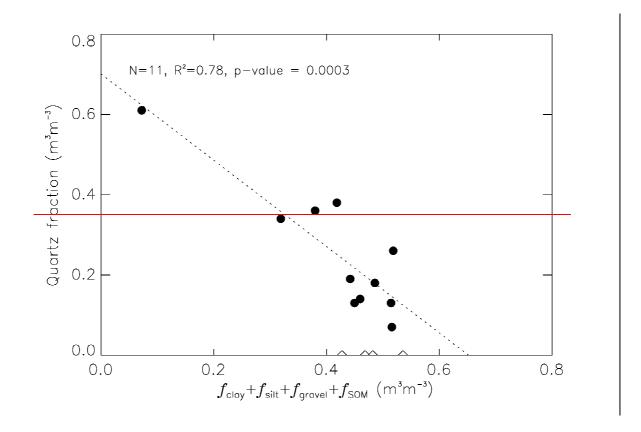


Fig. 5 – Non-null and null *q* retrievals (dark dots and opened diamonds, respectively) vs. the sum of clay, silt, gravel and SOM volumetric fractions (empirical Equation (12)).

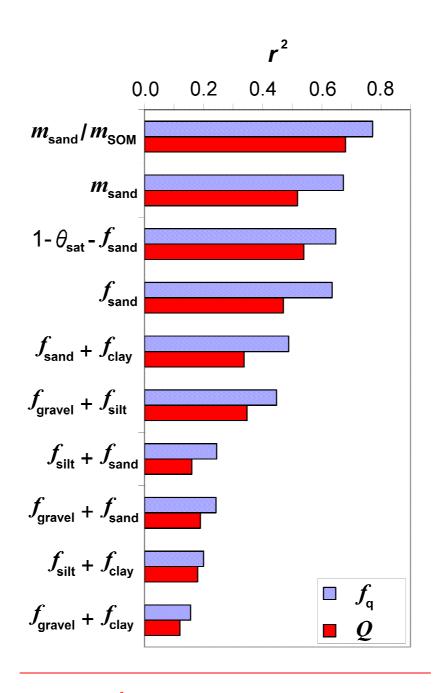


Fig. 4 – Fraction of variance (r^2) of gravimetric and volumetric fraction of quartz $(Q \text{ and } f_q, \text{ red and blue bars, respectively})$ explained by various predictors.

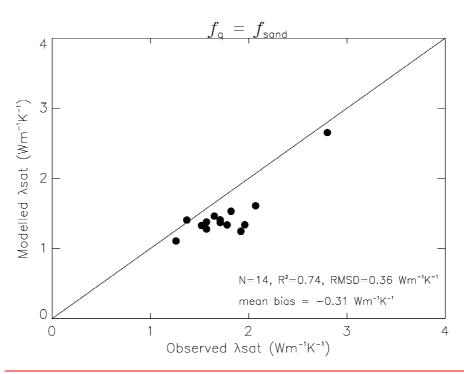


Fig. 5 – $\lambda_{\text{sat}MOD}$ values derived from volumetric quartz fractions f_{q} assumed equal to f_{sand} , using observed θ_{sat} values, vs. λ_{sat} retrievals.

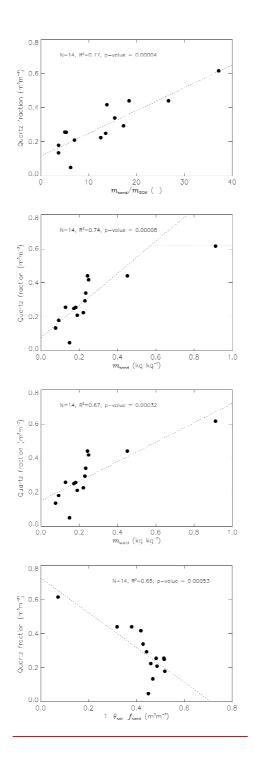


Fig. 6 – Pedotransfer functions for quartz: $f_{\rm q}$ retrievals (dark dots) vs. the four predictors of $f_{\rm q}$ given in Table 3. The modelled $f_{\rm q}$ values are represented by the dashed lines.

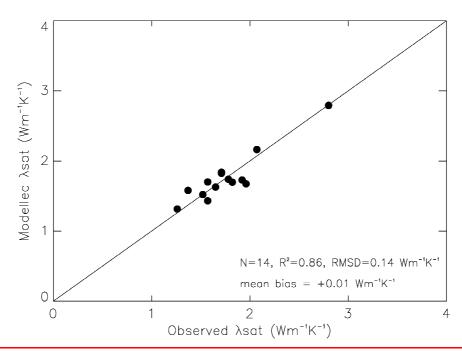
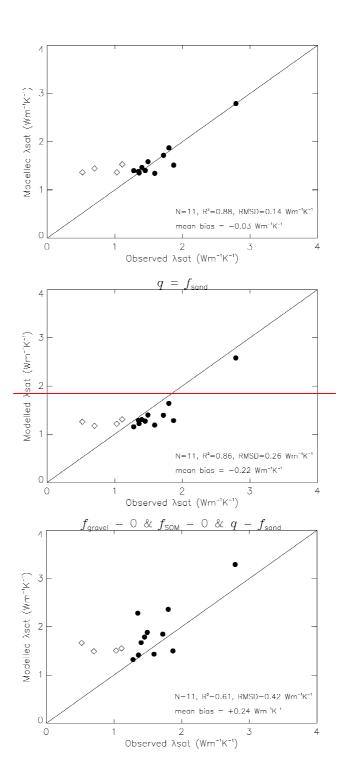


Fig. 7 – λ_{satMOD} values derived from the $m_{\text{sand}} / m_{\text{SOM}}$ pedotransfer function for the volumetric quartz fractions, using observed θ_{sat} values, vs. λ_{sat} retrievals.



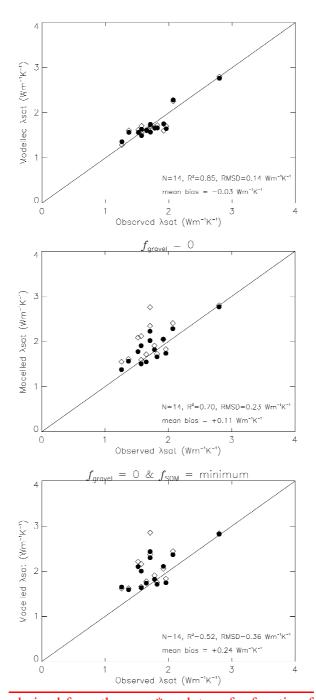
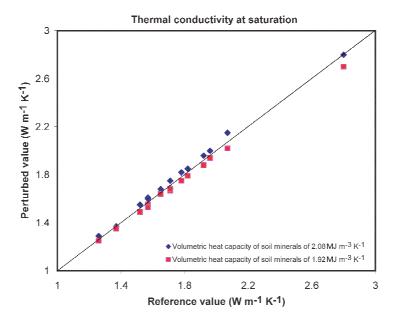


Fig. 86 – λ_{satMOD} values derived from the m_{sand}^* pedotransfer function for the volumetric quartz fractions, using θ_{satMOD} (Eqs. (13)) or the observed θ_{sat} (dark dots and opened diamonds, respectively), vs. λ_{sat} retrievals: (top) full model, (middle) $f_{\text{SOM}} = 0.013 \text{ m}^3 \text{m}^{-3}$, (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 θ_{satMOD} configuration. 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).





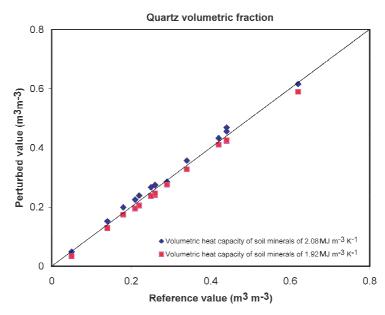
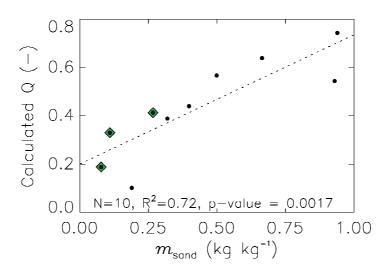


Fig. 9 – Impact of using values of $C_{\text{hmin}} = 1.92 \text{ MJ m}^{-3} \text{ K}^{-1}$ and $C_{\text{hmin}} = 2.08 \text{ MJ m}^{-3} \text{ K}^{-1}$ instead of $C_{\text{hmin}} = 2.0 \text{ MJ m}^{-3} \text{ K}^{-1}$ on (top) the retrieved λ_{sat} , (bottom) the volumetric fraction of quartz.



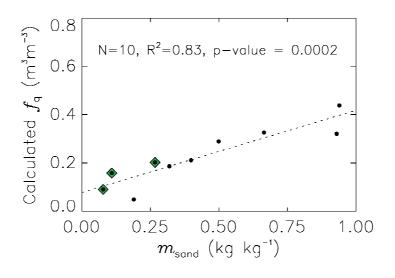
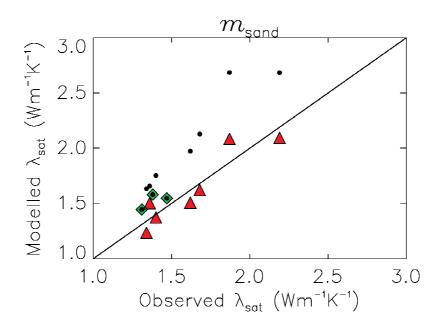


Fig. 10 – Gravimetric and volumetric fraction of quartz (top and bottom, respectively) derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) for 10 soils given by Tarnawski et al. (2009), vs. the gravimetric fraction of sand $m_{\rm sand}$. The three soils for which $m_{\rm sand}/m_{\rm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



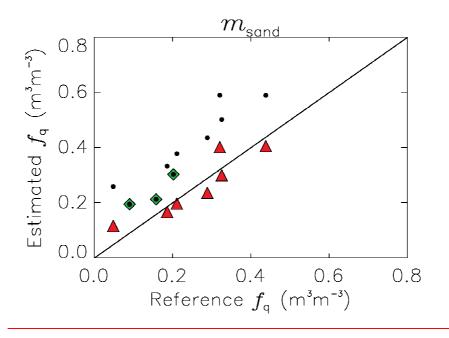


Fig. 11 – Estimated $\lambda_{\rm sat}$ and volumetric fraction of quartz $f_{\rm q}$ (top and bottom, respectively) vs. values derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) given by Tarnawski et al. (2009) for 10 Chinese soils, using the gravimetric fraction of sand $m_{\rm sand}$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

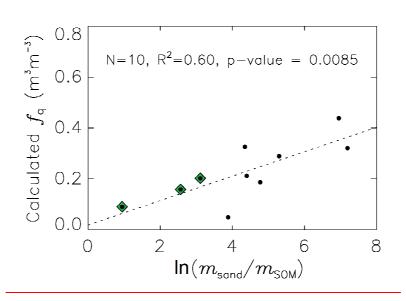


Fig. 12 – Volumetric fraction of quartz derived from the $\lambda_{\rm sat}$ observations of Lu et al. (2007) given by Tarnawski et al. (2009), vs. the logarithm of the $m_{\rm sand}/m_{\rm SOM}$ ratio. The three soils for which $m_{\rm sand}/m_{\rm SOM} < 40$ are indicated by green diamonds. The dashed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