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MEMORANDUM

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SUBJECT: FUMIGANT TRANSPORT MODELING WITH HYDRUS: ESTIMATION OF SOIL HYDRAULIC PARAMETERS USING PEDOTRANSFER FUNCTIONS

ABSTRACT

There are important differences between modeling the movement of nonvolatile chemicals in soil and volatile chemicals such as fumigants. For a nonvolatile chemical, convective transport (leaching) occurs in conjunction with water movement. The fastest rates of leaching occur when soil water content θ is high and soil pores are filled or nearly filled with water. In contrast, volatile solutes such as fumigants move primarily by diffusion in the vapor phase, and rates of volatile chemical movement are potentially highest at low θ, when air-filled porosities are correspondingly higher. Thus, while the impact of θ is important in both cases, accurate description of soil water content in the moderate to dry range is especially important for fumigant transport modeling.

To model changes in soil water content, knowledge of various soil-specific hydraulic parameters is required. Although soil hydraulic parameters can be measured, the procedures are difficult and time consuming. Alternately, estimation procedures have been developed that allow the parameters to be determined from easy to obtain soil properties, including textural composition and bulk density among others. The estimation procedures or algorithms are called pedotransfer functions (PTF). The vadose transport model HYDRUS (Šimůnek et al., 2008) includes several PTFs that a user may employ to estimate soil hydraulic characteristics. These PTFs are included for user convenience because soil hydraulic parameters are required as HYDRUS inputs. The PTFs were originally developed as part of a companion program named ROSETTA (Schaap et al., 1991). Similar to other PTFs, the ROSETTA PTFs were derived from soil databases containing several paired measurements of θ and soil water pressure head h for each of a large number of soils.

This report documents a modeling study to determine the effect of using PTF-estimated soil hydraulic parameters on HYDRUS-simulated fumigant volatilization. The PTF-based results were compared to simulations conducted with hydraulic parameters obtained directly from fitting to measured data. The results show that certain of the ROSETTA PTFs yield substantially

low-biased predicted θ as compared to experimentally measured $\theta(h)$, thereby also resulting in high-biased estimates of fumigant flux. Across 90 soils, median errors in PTF-derived cumulative nontarp emissions ranged up to 20 to 35 percent. The analysis also suggests a likely cause for the bias: the basis set of $\theta(h)$ data from which the PTFs were developed included many soils for which there was very limited or no data in the drier portion of the soil water retention curve. As a result, hydraulic parameters fitted to these limited data had large errors that translated into biased PTFs. The biases in the PTFs are probably less important at higher water contents, typically the primary region of interest for water and nonvolatile solute transport. This may explain why other modeling efforts have not identified this bias in the PTFs. The consequences for fumigant modeling, including calibration and validation are briefly discussed.

INTRODUCTION

First-principle vadose zone transport models such as LEACHM and HYDRUS typically simulate vapor phase transport of volatile solutes exclusively as a diffusion process. Diffusion coefficients in the gas phase are several orders of magnitude greater than in liquids. Consequently the rate of diffusive movement of a gas in a porous medium such as soil largely depends on the volume fraction of air-filled pores, in addition to pore geometry and the "interconnectedness" of those pores. In a given soil, the volume fraction of air-filled pores, their interconnectedness and associated gas diffusion path lengths are strongly dependent on water content. The net effect is that lower water contents yield faster rates of diffusion as compared to higher water contents.

Similar to other vadose zone transport programs, HYDRUS describes the effective gas phase diffusion coefficient D_e using a relationship based on work of Millington and Quirk (1961):

[1]
$$D_e = D_0 \tau_g$$

[2]
$$\tau_g = \frac{a_g^{7/3}}{\theta_s^2}$$

where D_0 is the diffusion coefficient in air, τ_g is the gas phase tortuosity factor, a_g is the gas-filled porosity and θ_s is the saturated volumetric water content, assumed equivalent to total porosity. With increasing water content both a_g and τ_g become smaller, causing a decrease in the effective diffusion coefficient D_e (Figure 1) and the rate of solute vapor-phase movement. Practically speaking, this means that accurate modeling of fumigant transport in soils depends on accurate simulation of water content.

The Richards equation is used to accurately model water movement in virtually all reputable unsaturated zone models. Numerical solutions to that nonlinear partial differential equation require knowledge of the relationship between pressure head h and water content θ. As pressure head h becomes increasingly negative, water content θ decreases. The relationship between h and θ is called the soil-water retention function. Various empirical relationships have been developed throughout the years to describe soil-water retention functions with the van Genuchten (1980) retention function being one of the most commonly used. That $\theta(h)$ relationship is:

[3]
$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + |\alpha h|^n)^{1-1/n}}$$

where

S_e = effective water content (dimensionless, range 0 – 1)
θ_s = saturated water content (cm^3 water/cm^3 bulk soil)
θ_r = residual water content (cm^3 water/cm^3 bulk soil)
h = soil water pressure head (cm), ≤ 0
α, n – empirical parameters (cm^{-1} and dimensionless, respectively)

In this paper, θ_s, θ_r, α, and n are referred to as van Genuchten soil hydraulic parameters, or simply as VG parameters. The parameters θ_s and θ_r are the saturated and residual water contents, respectively. The residual water content may be thought of as the limiting water content as soil water pressure head approaches very high negative values (van Genuchten, 1980). In practice, due to the asymptotic nature of θ_r, it is better considered a fitting parameter as opposed to assigning any physical meaning (van Genuchten and Nielsen, 1985; M. Schaap. personal communication). While θ_s can be measured directly, θ_r, α, and n are obtained by fitting to experimental $\theta(h)$ data. However, the experimental measurements are difficult and time consuming. Alternately, PTFs have been developed to estimate the four VG hydraulic parameters from soil properties. Schaap et al. (1998) used a neural network procedure to develop several PTFs using $\theta(h)$ data for 1206 soils. Those PTFs included various explanatory variables, including textural class, sand, silt, and clay percentage, bulk density, $\theta_{1/3}$ and θ_{15}. The latter variables are soil water content at -⅓ bar and -15 bar pressure head (h = -333 cm and -15000 cm, respectively). The parameters $\theta_{1/3}$ and θ_{15} have traditionally been considered as the soil-water content at field capacity and permanent wilting point, respectively. Schaap et al. (1998) reported that, generally, those PTFs based on a greater number of variables yielded parameter estimates that were in better agreement with those obtained from experimental $\theta(h)$ data.

Subsequently Schaap et al. (2001) expanded that work by developing ROSETTA (available for download *at*: <http://cals.arizona.edu/research/ROSETTA/download/ROSETTA.pdf>). ROSETTA is a hierarchical parameter estimation program that allows the user simple or more complex PTF choices depending on soil input data availability. They developed the program using neural network and bootstrap techniques from retention data for > 2000 soils. ROSETTA includes five different PTFs for estimating soil hydraulic parameters from soils data (Table 1). A simplified version of the program is included as a module in HYDRUS1-D and HYDRUS2/3D. The ROSETTA PTFs are the most comprehensive PTFs available for predicting soil VG parameters.

The simplest PTF proposed by Schaap et al. (2001) consists of a lookup table of mean θ_s, θ_r, α, and n for each soil textural class (PTF#1, Table 1). This model has the obvious advantage that measurement of site-specific soil properties may not be required–for example, the soil textural class for a specific location may be determined from soil survey data. In evaluating goodness of fit of various PTFs, Schaap et al. (1998) reported that a simple PTF model based on textural means, similar to PTF#1, yielded predicted hydraulic parameters that agreed only poorly with those obtained by fitting Eq. 3 to $\theta(h)$ data. The next two PTFs (PTF#2 and #3, Table 1) require specific soil data that are relatively easy to measure: sand, silt and clay content (PTF#2), and bulk density (PTF#3). The last two PTFs also include $\theta_{1/3}$ (PTF#4) and θ_{15} (PTF#5) as additional explanatory variables, and have been reported to generally yield the best hydraulic parameter predictions (Schaap et al., 2001).

OBJECTIVE

The objective of this analysis is to determine the effect of the different PTFs available in ROSETTA on simulated fumigant flux ratios. The effect of the PTFs (Table 1) were evaluated by comparing simulated fumigant flux ratios obtained using each PTF to simulated flux ratios obtained using VG parameters estimated directly from experimental $\theta(h)$ data.

METHODS

Modeling Overview

All simulations were conducted using HYDRUS 1-D (Šimůnek et al., 2008). Two fumigant simulation scenarios were used to evaluate the effect of choice of PTF on model output: a broadcast tarp 1,3-dichloropropene (1,3-D) application and a broadcast no tarp 1,3-D application. Each scenario was simulated 6 different times in each of 90 soils. One of those simulations utilized VG hydraulic parameters fitted from measured $\theta(h)$ data as model inputs, while the other five simulations were conducted using inputs of estimated VG parameters from each of the five PTFs (Table 1). The 90 soils fell in 4 different soil textural classes: loam (22 soils), sandy loam (27 soils), loamy sand (16 soils), and sand (25 soils). Other soil types were deemed unlikely to receive 1,3-D applications in California so were not studied here. Both application scenarios were modeled using an initial uniform 1,3-D distribution in the soil over a depth of 30–45 cm

(12 inches–18 inches). The uniform soil profile was 150 cm deep, the initial soil-water condition was a constant pressure head h = -500cm, and the simulations were for a 21 day duration. The presence of a tarp was simulated by increasing the surface boundary layer thickness from the 0.5 cm default to 150 cm, thus increasing mass transfer resistance at the soil surface. The untarped scenario included two 0.6 cm post-application irrigations on day one and day two. Preliminary simulations were conducted to determine the number and distribution of nodes in the profile required to achieve solute mass errors < 1 percent. Flux ratios were calculated as total cumulative emissions over the 21 day period divided by total fumigant applied. Additional parameter estimates used in the simulations are given in Appendix 1.

Soil selection

Soil texture classification, percent sand, percent silt, percent clay, bulk density and $\theta(h)$ data were obtained from the Unsaturated Soil Hydraulic Database (UNSODA, Leij et al., 1996). The 90 soils were selected from a total of 321 sands, loamy sands, sandy loams and loams in UNSODA. Two conditions based on the range of $\theta(h)$ data were required for a soil to be chosen: (1) maximum $h \geq$ -1 cm, and (2) minimum $h \leq$ -15000 cm. These conditions were imposed to so that only soils with a broad range in $\theta(h)$ were obtained, reducing the error associated with estimating VG hydraulic parameters from a limited range of $\theta(h)$ data. The VG parameters were estimated by fitting the experimental $\theta(h)$ data for each soil to Equation 3 using the nonlinear optimization program RETC (van Genuchten et al., 1991).

Saturated Hydraulic Conductivities

Saturated hydraulic conductivity K_s data are required as inputs for HYDRUS, but those data were not available for most of the soils. Consequently K_s estimates were obtained from sand, silt, and clay percentages, bulk density, $\theta_{1/3}$ and θ_{15} data using ROSETTA (Schaap et al., 2001). Total water fluxes out of the profile were generally very small. A brief sensitivity analysis showed essentially no effect of K_s on flux ratio for the tarped scenario here. The effect of varying K_s over an order of magnitude in the untarped scenario did result in small changes in flux ratio, typically on the order of a few percent. Given the low water inputs into the profile, constant initial pressure head with depth, very low bottom and top boundary water fluxes, and the unsaturated soil conditions during the simulations, the effect on simulated flux ratios due to estimating K_s as opposed to measuring that parameter was deemed minor.

RESULTS

Fitted and PTF#1–Estimated VG Parameters

Example RETC fits of Equation 3 are shown in Figure 2. The texture class mean fitted parameters for the 90 selected UNSODA soils were significantly different than the means comprising ROSETTA PTF#1 in some cases (Table 2). The ROSETTA PTF#1 averages for the four texture classes were obtained by fitting Equation 3 to $\theta(h)$ data of 1243 soils from 3 large databases (Schaap and Leij, 1998). Data for 26 percent of those soils (321 soils) came from the UNSODA database. Although only 90 of the 321 UNSODA soils met the pressure head screening criteria in this study (maximum $h \geq -1$ cm and minimum $h \leq -15000$ cm), all 321 UNSODA soils in the four texture groups were included in calculation of ROSETTA's PTF#1 textural means (Schaap et al., 2001). Thus, most of the UNSODA fitted VG parameters used to estimate PTF#1 texture class means were derived from $\theta(h)$ data measured over limited ranges of pressure head; more than half of the UNSODA soil $\theta(h)$ data sets had minimum soil water pressure heads h >-1000cm (Figure 3).

Estimates of θ_r derived from fits to limited ranges of $\theta(h)$ data are sometimes unrealistic (Figure 4). The fitted parameters for the two soils in Figure 4 were among those used to calculate the textural class parameter means comprising ROSETTA PTF#1. Across all 321 Sand–Loam UNSODA soils, estimated θ_r from such limited $\theta(h)$ data are significantly greater than when estimates were derived from a broader range of $\theta(h)$ data, regardless of soil textural class (analysis of variance, p<0.001; Appendix 2). Moreover, in nearly all cases, when high values of θ_r are observed, the $\theta(h)$ data from which those estimate were obtained only include $\theta(h)$ measurements in the "wetter" range (e.g. where minimum $h > -1000$ cm) (Appendix 2).

Carsel and Parrish (1985) and Tietje (1999) recognized the importance of a potential covariance structure of the VG parameters. Across the 90 soils here, the correlation between θ_r and log(n) is significant (r = 0.45, p<0.001; Figure 5). This means that bias in estimates of one (e.g. θ_r) may also be associated with bias or error in estimates of the other (log(n)). While Figure 4 demonstrates grossly unrealistic θ_r, estimates for the fitted empirical shape parameter n are quite high (*cf.* Table 2). Analysis of all 321 UNSODA soils yields very similar results as observed for θ_r: estimates of the shape parameter n are significantly greater when $\theta(h)$ data over a limited range (i.e. the "wet" range, minimum $h > -1000$ cm) are used to fit Equation 3 (analysis of variance, p<0.001; Appendix 2). Thus, retention functions derived from limited $\theta(h)$ are generally characterized by high-biased estimates of both θ_r and n. Finally, all other things being equal, Figure 6 illustrates the effect of increasing n: large values of n result in retention curves wherein θ approaches θ_r at lower soil water pressure heads.

Soil water retention functions calculated from fitted VG parameters were variable within each textural class (Figure 7). However, the expected general trend of increased "tailing" for finer textured soils as compared to coarser soils was evident. For example, none of the loam retention curves approached their horizontal asymptotic water content θ_r in the interval -1000 cm > h > -10000 cm. In contrast, several of the sands reached essentially constant water content within that range (Figure 7). Soil water retention functions calculated from the PTF#1 textural class means deviated markedly from those calculated from fitted VG parameters (Figure 7). In general, the PTF#1-based retention curves approached the asymptotic θ_r much sooner (at much less negative h) as compared to retention curves calculated from the fitted VG parameters (Figure 7). This is consistent with the behavior one would expect if the PTF#1 estimates of the parameter n were high biased.

Observed versus PTF Estimated Water Contents

There were a total of 983 observed $\theta(h)$ data for the 90 soils. Predicted $\theta(h)$ data were calculated using Equation 3 and (a) fitted VG parameters and (b) VG parameters estimated from each of the five different PTFs in Table 1. The retention functions based on the fitted VG parameters fit the observed water contents well, with a correlation between predicted and observed water contents of 0.996 (Figure 8). In contrast, all of the PTF-based predictions showed systematic deviations between predicted and observed water contents: PTF-based retention function predictions were consistently lower than observed water contents. Similar to the findings of Schaap et al. (2001), the more complex PTFs based on more soil information yielded better agreement with fitted data. The error in predicted water contents of the retention function based on PTF#1 was particularly striking, with a mean absolute deviation of > 8 percent (percent deviation = [(fitted – observed)/observed] * 100). The systematic under-prediction of water contents by PTFs implies that calculated τ_g (Equation 2), and correspondingly D_e (effective diffusion coefficient, Equation 1) will be generally higher when PTFs are used to estimate VG parameters as opposed to τ_g calculated from VG parameters that are determined from measured $\theta(h)$ data.

Effect of PTFs on Simulated Emissions

Simulations based on fitted VG parameters and those based on the various PTFs showed qualitatively similar effect of tarping and effect of soil texture on fumigant flux ratios. In general, the no tarp applications had greater flux ratios than the tarped scenario, and median flux ratios were greater in coarse soils (Figures 9,10; Tables 3, 4).

The flux ratios obtained using different PTFs were evaluated by comparison to ratios obtained using fitted VG parameters. Thus, simulations using fitted VG parameters were treated as a standard, or control, for each set of PTF simulations conducted on a particular soil with a given tarp scenario. For each simulation, the difference in flux ratio between the simulation and the control was calculated as *flux difference* = (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$) (Figures 11,12).

For nearly all combinations of soil texture, PTF and simulation scenario, median flux differences were greater than zero (Figure 13). The only exceptions were for nontarped simulations in sand where median differences for PTF#3, PTF#4, and PTF#5 were small but negative (Tables 5,6). In several other cases median differences were greater than zero, and the overestimation effect of was particularly strong for loam soils in the untarped scenario (Figure 11). The textural mean PTF#1 showed the greatest deviation from the fitted VG simulations, where median differences in no tarp and tarp scenarios for Sandy Loams and Loams ranged from 25 to 34 percent (Tables 5, 6; Figure 13). In the coarser sand and loamy sand soil textures, the textural mean-based PTF yielded median flux ratio differences of 5 to 6 percent, although the upper 75th and 90th percentiles were in the general range of 10 – 30 percent for sand and loamy sand soils.

DISCUSSION

The fitted versus observed water content data and fumigant modeling results show consistent effects: the PTFs generally underestimate $\theta(h)$, leading to higher than expected τ_g and generally high-biased simulated flux ratios. The low PTF-predicted $\theta(h)$ and high PTF-based simulated flux ratios are least partially a result of bias in the fitted VG parameters used to originally develop the PTFs.

Although it could be argued that such a conservative (high) bias in simulated flux ratios is acceptable (or even desirable) when estimating exposures, the consistent bias is problematic from a model validation standpoint. One purpose of model validation is to define a parameter space, or set of environmental conditions, over which a model accurately describes reality. Consequently a substantial and consistent bias in flux ratio means that, by definition, a model cannot be validated. This is true regardless of whether the simulated flux ratio is too high or too low.

Any systematic deviations in flux ratio attributable to PTFs also creates difficulties in model calibration. Accurate simulation of fumigant volatilization necessarily includes complex mathematical description of several complex linked processes, including sorption, degradation, diffusion, water retention and movement, temperature effects, and mass transfer into and out of the surface boundary layer. Calibration generally involves identifying “best-fit” values of unknown input parameters, such as degradation rate constants or sorption coefficients. Best-fit or optimal parameter values are typically identified by minimizing some objective function such as the sum of squared deviations between observed and simulated data. It is evident that optimizing agreement between observed data and (biased) modeled flux ratios may very well force changes in other parameters to compensate for the bias. For example, calibrating a biased model may yield "calibrated" degradation rate constant that does not reflect actual degradation in the field – effectively defeating the purpose of site-specific calibration.

CONCLUSION

The weakest aspect of most PTFs is their prediction of residual water content θ_r (M. Schaap, personal communication, 2008). For example, the correlations between observed and fitted θ_r for ROSETTA range from 0.07 (PTF#1) to 0.39 (PTF#5) (Schaap et al., 2001). Liquid-phase transport occurs predominately at higher water contents, so this characteristic of PTFs may be a relatively minor concern in situations where water or dissolved solute movement is of interest. However, the opposite is true of fumigant transport: diffusive gas-phase transport is greatest at lowest water contents. Thus, accurately characterizing the soil-water retention function at intermediate-to-low water contents is critical for accurately simulating fumigant transport.

Based on the simulation results here, the use of ROSETTA's textural average PTF#1 in fumigant modeling should be avoided. The PTF#1-based predictions were in poor agreement with observed water content data (Figure 8) and also yielded high-biased flux ratios (Tables 5 and 6). These results are at least partially attributable to the systematic bias in θ_r and n when these parameters are estimated from limited ranges of $\theta(h)$ data (e.g. when minimum $h > -1000$ cm).

While PTF#2 and PTF#3 yield very similar differences in flux ratios in both tarped and untarped scenarios (Tables 5 and 6), the systematic deviation of PTF#2 predicted water contents from observed values at high water contents (Figure 8) argues against the use of PTF#2 relative to PTF#3. As noted previously, only minimal water movement occurred in the two scenarios studied here, likely explaining the similar performance of the two PTFs when compared on the basis of simulated flux ratios obtained here. In other scenarios where water movement is important, PTF#3 may be the better choice due to a somewhat better correlation between observed and predicted water contents. Finally, the additional data required for PTF#3 as compared to PTF#2 is soil bulk density; an easy and inexpensive characteristic to measure.

PTF#4 and PTF#5 performed relatively well in the tarped scenario, yielding modest 75th to 90th percentile differences between PTF-derived flux ratios and fitted VG parameter-derived ratios on the order of 5 to 10 percent fumigant volatilized (Table 6). However, the deviations for the nontarp scenario were substantially greater, generally approaching 20 percent fumigant volatilized in some cases. Thus, with the possible exception of sands (Table 5), a rigorous validation of HYDRUS in an untarped scenario may require measurement of $\theta(h)$ data over a wide range in soil-water pressure head. Estimated VG parameters can then be obtained by fitting Equation 3 to the measured data.

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Table 1. ROSETTA pedotransfer functions.

PTF	Required Input Data
#1	soil texture – PTF based on texture class means of fitted VG parameters
#2	sand, silt and clay content (percent)
#3	same as 2 above, plus soil bulk density
#4	same as 3 above, plus -1/3 bar volumetric water content
#5	same as 4 above, plus -15 bar volumetric water content

Table 2. Means comparisons (within textural class) between ROSETTA PTF#1 VG parameter texture class means (θ_r , θ_S , $\log_{10}(\alpha)$ and $\log_{10}(n)$) and fitted VG parameter means determined here for 90 UNSODA soils. Statistical measures (N, mean, standard deviation = s.d.) for PTF#1 as reported by Schaap et al. (2001); statistical measures for the 90 UNSODA soils in four textural classes calculated from fitted data here.

data source	**Texture Class**	**N**	**mean θ_r**	***s.d.***	**significant difference‡**
PTF#1	Loam	242	0.061	0.073	sig
PTF#1	LoamySand	201	0.049	0.042	ns
PTF#1	Sand	308	0.053	0.029	sig
PTF#1	SandyLoam	476	0.039	0.054	ns
UNSODA Fits	Loam	22	0.013	0.042	---
UNSODA Fits	LoamySand	16	0.044	0.034	---
UNSODA Fits	Sand	25	0.033	0.024	---
UNSODA Fits	SandyLoam	27	0.036	0.041	---
			mean θ_S	***s.d.***	
PTF#1	Loam	242	0.399	0.098	sig
PTF#1	LoamySand	201	0.390	0.070	ns
PTF#1	Sand	308	0.375	0.055	ns
PTF#1	SandyLoam	476	0.387	0.085	ns
UNSODA Fits	Loam	22	0.476	0.117	---
UNSODA Fits	LoamySand	16	0.421	0.061	---
UNSODA Fits	Sand	25	0.374	0.050	---
UNSODA Fits	SandyLoam	27	0.394	0.067	---
			mean $\log_{10}(\alpha)$	***s.d.***	
PTF#1	Loam	242	-1.954	0.730	sig
PTF#1	LoamySand	201	-1.459	0.470	ns
PTF#1	Sand	308	-1.453	0.250	ns
PTF#1	SandyLoam	476	-1.574	0.560	sig
UNSODA Fits	Loam	22	-1.331	0.588	---
UNSODA Fits	LoamySand	16	-1.310	0.359	---
UNSODA Fits	Sand	25	-1.508	0.330	---
UNSODA Fits	SandyLoam	27	-1.781	0.435	---
			mean $\log_{10}(N)$	***s.d.***	
PTF#1	Loam	242	0.168	0.130	sig
PTF#1	LoamySand	201	0.242	0.160	ns
PTF#1	Sand	308	0.502	0.180	sig
PTF#1	SandyLoam	476	0.161	0.110	ns
UNSODA Fits	Loam	22	0.061	0.014	---
UNSODA Fits	LoamySand	16	0.207	0.092	---
UNSODA Fits	Sand	25	0.298	0.134	---
UNSODA Fits	SandyLoam	27	0.145	0.102	---

‡ Significant differences by textural class based on two sample t-test with unequal variances. ns=not significant, sig=significant, $p< 0.05$.

Table 3. Percentiles of simulated flux ratios by VG parameter estimation method and textural class for "No Tarp" scenario.

Simulation scenario	VG parameter source	textural class	minimum	10th percentile	25th percentile	median	75th percentile	90th percentile	maximum
No Tarp	VGFitted	Sand	0.360	0.427	0.473	0.538	0.570	0.597	0.623
No Tarp	PTF #1	Sand				0.607			
No Tarp	PTF #2	Sand	0.530	0.535	0.547	0.553	0.564	0.570	0.591
No Tarp	PTF #3	Sand	0.448	0.503	0.523	0.547	0.578	0.589	0.599
No Tarp	PTF #4	Sand	0.352	0.428	0.482	0.502	0.566	0.570	0.600
No Tarp	PTF #5	Sand	0.300	0.362	0.458	0.521	0.566	0.583	0.594
No Tarp	VGFitted	LoamySand	0.005	0.108	0.424	0.508	0.533	0.545	0.557
No Tarp	PTF #1	LoamySand				0.559			
No Tarp	PTF #2	LoamySand	0.480	0.486	0.499	0.512	0.543	0.559	0.564
No Tarp	PTF #3	LoamySand	0.439	0.490	0.500	0.521	0.556	0.583	0.585
No Tarp	PTF #4	LoamySand	0.130	0.273	0.471	0.513	0.563	0.581	0.586
No Tarp	PTF #5	LoamySand	0.193	0.333	0.428	0.534	0.563	0.579	0.583
No Tarp	VGFitted	SandyLoam	0.004	0.056	0.107	0.246	0.328	0.487	0.506
No Tarp	PTF #1	SandyLoam				0.511			
No Tarp	PTF #2	SandyLoam	0.244	0.247	0.290	0.327	0.388	0.426	0.462
No Tarp	PTF #3	SandyLoam	0.078	0.214	0.260	0.303	0.410	0.446	0.496
No Tarp	PTF #4	SandyLoam	0.107	0.119	0.149	0.237	0.382	0.423	0.550
No Tarp	PTF #5	SandyLoam	0.023	0.045	0.146	0.266	0.399	0.459	0.509
No Tarp	VGFitted	Loam	0.000	0.000	0.001	0.021	0.117	0.285	0.298
No Tarp	PTF #1	Loam				0.359			
No Tarp	PTF #2	Loam	0.201	0.218	0.238	0.243	0.250	0.273	0.284
No Tarp	PTF #3	Loam	0.096	0.101	0.219	0.275	0.318	0.339	0.351
No Tarp	PTF #4	Loam	0.048	0.058	0.166	0.209	0.258	0.282	0.318
No Tarp	PTF #5	Loam	0.010	0.064	0.097	0.191	0.281	0.350	0.398

Table 4. Percentiles of simulated flux ratios by VG parameter estimation method and textural class for "Tarp" scenario.

Simulation scenario	VG parameter source	textural class	minimum	10th percentile	25th percentile	median	75th percentile	90th percentile	maximum
Tarp	VGFitted	Sand	0.133	0.225	0.303	0.343	0.365	0.394	0.408
Tarp	PTF #1	Sand				0.400			
Tarp	PTF #2	Sand	0.357	0.367	0.372	0.376	0.380	0.384	0.394
Tarp	PTF #3	Sand	0.313	0.340	0.362	0.373	0.384	0.387	0.387
Tarp	PTF #4	Sand	0.175	0.305	0.325	0.357	0.375	0.383	0.390
Tarp	PTF #5	Sand	0.145	0.192	0.321	0.347	0.378	0.390	0.392
Tarp	VGFitted	LoamySand	0.003	0.063	0.235	0.316	0.343	0.354	0.360
Tarp	PTF #1	LoamySand				0.377			
Tarp	PTF #2	LoamySand	0.306	0.312	0.323	0.335	0.362	0.372	0.374
Tarp	PTF #3	LoamySand	0.295	0.311	0.322	0.344	0.363	0.376	0.377
Tarp	PTF #4	LoamySand	0.044	0.087	0.303	0.351	0.356	0.378	0.379
Tarp	PTF #5	LoamySand	0.109	0.169	0.263	0.347	0.359	0.378	0.380
Tarp	VGFitted	SandyLoam	0.000	0.000	0.003	0.088	0.190	0.284	0.338
Tarp	PTF #1	SandyLoam				0.349			
Tarp	PTF #2	SandyLoam	0.117	0.117	0.135	0.178	0.223	0.259	0.292
Tarp	PTF #3	SandyLoam	0.025	0.103	0.135	0.163	0.238	0.267	0.314
Tarp	PTF #4	SandyLoam	0.008	0.013	0.037	0.096	0.220	0.242	0.365
Tarp	PTF #5	SandyLoam	0.003	0.008	0.053	0.130	0.248	0.282	0.349
Tarp	VGFitted	Loam	0.000	0.000	0.000	0.007	0.078	0.169	0.203
Tarp	PTF #1	Loam				0.249			
Tarp	PTF #2	Loam	0.060	0.067	0.072	0.092	0.109	0.114	0.125
Tarp	PTF #3	Loam	0.030	0.036	0.086	0.102	0.119	0.138	0.140
Tarp	PTF #4	Loam	0.005	0.010	0.020	0.055	0.072	0.105	0.123
Tarp	PTF #5	Loam	0.002	0.023	0.038	0.096	0.134	0.182	0.199

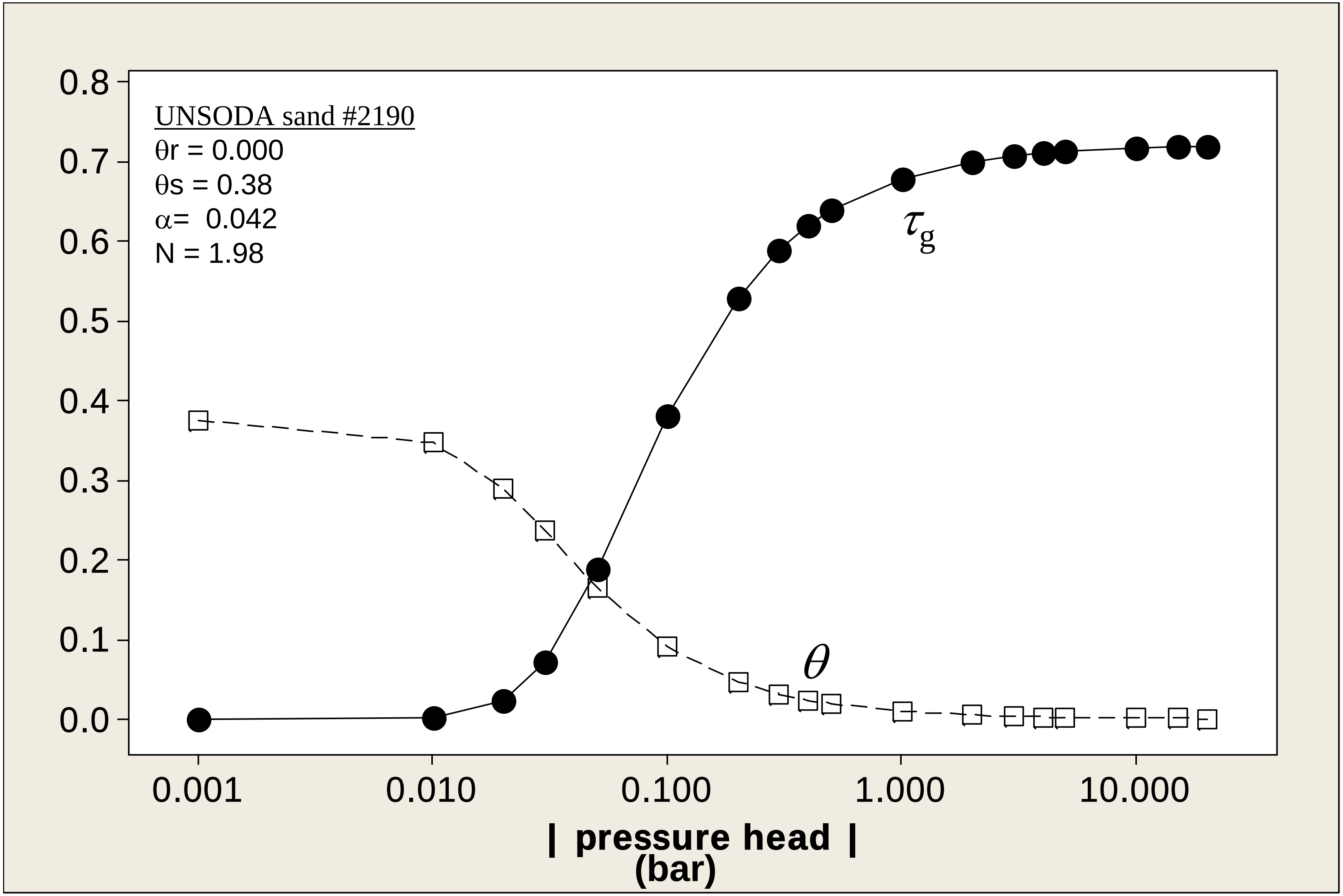
Table 5. Flux ratio differences by PTF and textural class for "No Tarp" scenario. Differences calculated as (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$).

Simulation scenario	PTF	textural class	minimum	10th percentile	25th percentile	median	75th percentile	90th percentile	maximum
No Tarp	PTF #1	Sand	-0.016	0.009	0.037	0.068	0.134	0.180	0.246
No Tarp	PTF #2	Sand	-0.063	-0.031	-0.019	0.002	0.090	0.164	0.202
No Tarp	PTF #3	Sand	-0.080	-0.050	-0.040	-0.007	0.073	0.144	0.224
No Tarp	PTF #4	Sand	-0.076	-0.052	-0.045	-0.008	0.024	0.071	0.144
No Tarp	PTF #5	Sand	-0.117	-0.061	-0.039	-0.021	0.000	0.020	0.074
No Tarp	PTF #1	LoamySand	0.002	0.014	0.026	0.051	0.136	0.451	0.554
No Tarp	PTF #2	LoamySand	-0.058	-0.048	-0.022	0.023	0.114	0.389	0.501
No Tarp	PTF #3	LoamySand	-0.052	-0.039	-0.006	0.043	0.114	0.434	0.443
No Tarp	PTF #4	LoamySand	-0.036	-0.023	0.003	0.038	0.066	0.124	0.166
No Tarp	PTF #5	LoamySand	-0.082	-0.005	0.012	0.026	0.051	0.188	0.226
No Tarp	PTF #1	SandyLoam	0.005	0.024	0.183	0.265	0.404	0.455	0.508
No Tarp	PTF #2	SandyLoam	-0.084	-0.046	0.019	0.077	0.183	0.250	0.337
No Tarp	PTF #3	SandyLoam	-0.091	-0.055	0.010	0.073	0.144	0.212	0.337
No Tarp	PTF #4	SandyLoam	-0.108	-0.064	-0.022	0.018	0.074	0.099	0.256
No Tarp	PTF #5	SandyLoam	-0.128	-0.071	-0.042	0.010	0.088	0.142	0.245
No Tarp	PTF #1	Loam	0.061	0.074	0.242	0.338	0.358	0.359	0.359
No Tarp	PTF #2	Loam	-0.084	-0.013	0.137	0.207	0.240	0.242	0.265
No Tarp	PTF #3	Loam	0.019	0.052	0.076	0.181	0.251	0.284	0.318
No Tarp	PTF #4	Loam	-0.020	0.008	0.047	0.145	0.168	0.192	0.257
No Tarp	PTF #5	Loam	-0.038	0.048	0.064	0.121	0.173	0.184	0.257

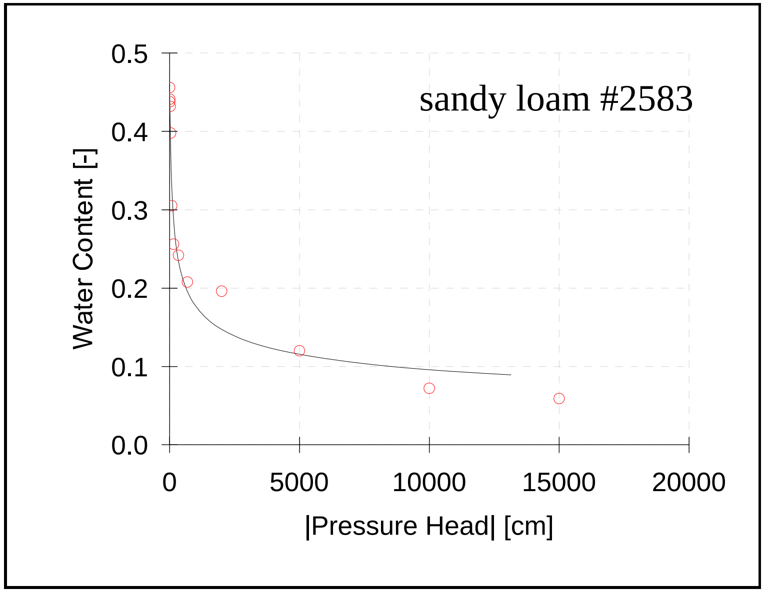
Table 6. Flux ratio differences by PTF and textural class for "Tarp" scenario. Differences calculated as (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$).

Simulation scenario	PTF	textural class	minimum	10th percentile	25th percentile	median	75th percentile	90th percentile	maximum
Tarp	PTF #1	Sand	-0.008	0.006	0.035	0.057	0.096	0.174	0.266
Tarp	PTF #2	Sand	-0.029	-0.017	0.008	0.037	0.072	0.147	0.244
Tarp	PTF #3	Sand	-0.034	-0.032	-0.006	0.020	0.084	0.140	0.248
Tarp	PTF #4	Sand	-0.038	-0.032	-0.010	0.016	0.045	0.066	0.086
Tarp	PTF #5	Sand	-0.063	-0.023	-0.012	0.011	0.022	0.040	0.054
Tarp	PTF #1	LoamySand	0.016	0.022	0.034	0.060	0.142	0.313	0.373
Tarp	PTF #2	LoamySand	-0.046	-0.029	-0.012	0.023	0.120	0.258	0.326
Tarp	PTF #3	LoamySand	-0.037	-0.023	-0.004	0.030	0.129	0.283	0.292
Tarp	PTF #4	LoamySand	-0.009	0.003	0.018	0.026	0.039	0.060	0.107
Tarp	PTF #5	LoamySand	-0.025	-0.002	0.008	0.027	0.048	0.106	0.106
Tarp	PTF #1	SandyLoam	0.011	0.065	0.159	0.261	0.346	0.349	0.349
Tarp	PTF #2	SandyLoam	-0.047	-0.029	0.018	0.090	0.122	0.150	0.237
Tarp	PTF #3	SandyLoam	-0.027	-0.026	0.019	0.095	0.126	0.150	0.238
Tarp	PTF #4	SandyLoam	-0.068	-0.033	-0.001	0.013	0.031	0.047	0.154
Tarp	PTF #5	SandyLoam	-0.016	0.003	0.005	0.035	0.053	0.112	0.159
Tarp	PTF #1	Loam	0.046	0.080	0.170	0.242	0.249	0.249	0.249
Tarp	PTF #2	Loam	-0.121	-0.091	0.025	0.063	0.094	0.109	0.123
Tarp	PTF #3	Loam	-0.105	-0.043	0.030	0.064	0.086	0.115	0.130
Tarp	PTF #4	Loam	-0.097	-0.088	-0.007	0.015	0.039	0.042	0.061
Tarp	PTF #5	Loam	-0.034	-0.005	0.014	0.040	0.057	0.082	0.108

Figure 1. Example plot of calculated soil-water content θ and gas phase tortuosity τ_g vs. <u>absolute</u> value of soil-water pressure head (bars). Calculated using Equations 1 and 2.



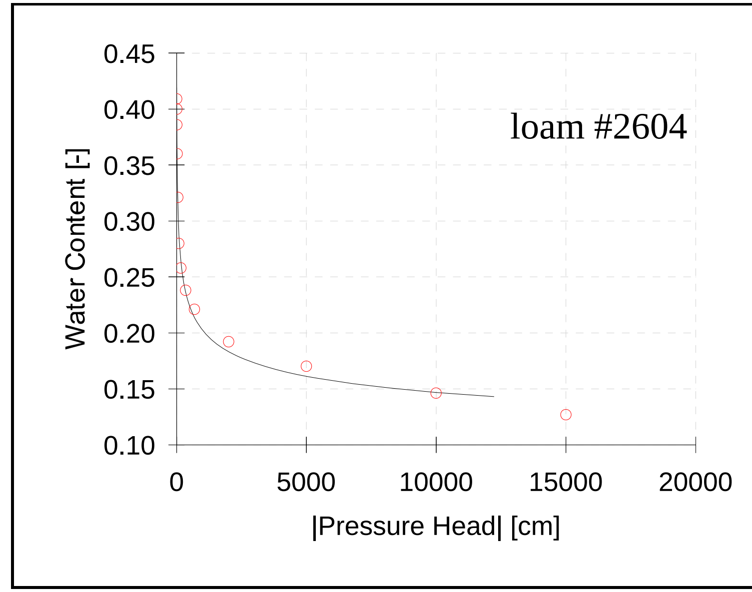
Hydraulic Properties: Theta vs. h



θ_r	θ_s	α	n
0.00	0.46	0.035	1.268

R^2 fitted vs obs = 0.97

Hydraulic Properties: Theta vs. h

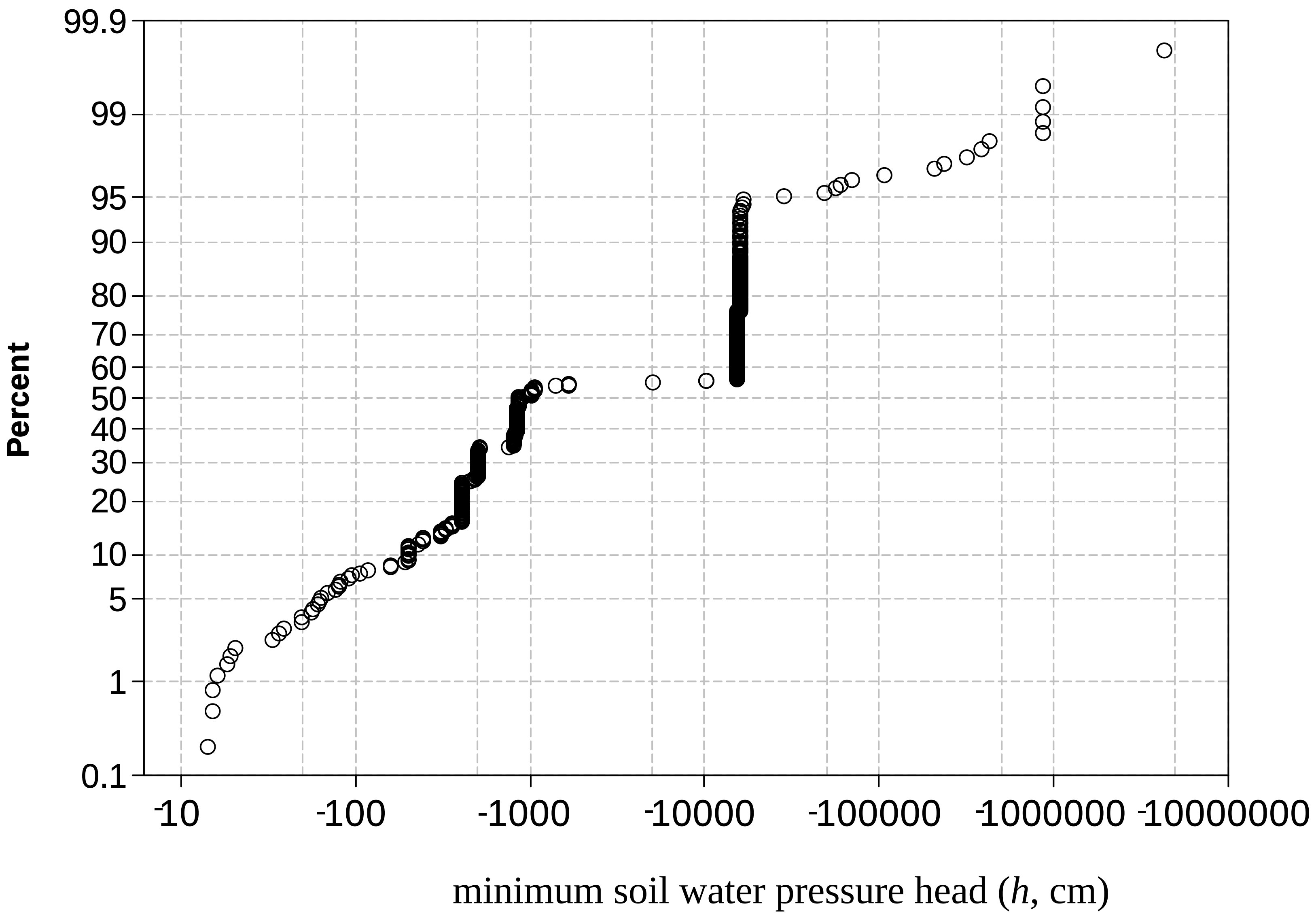


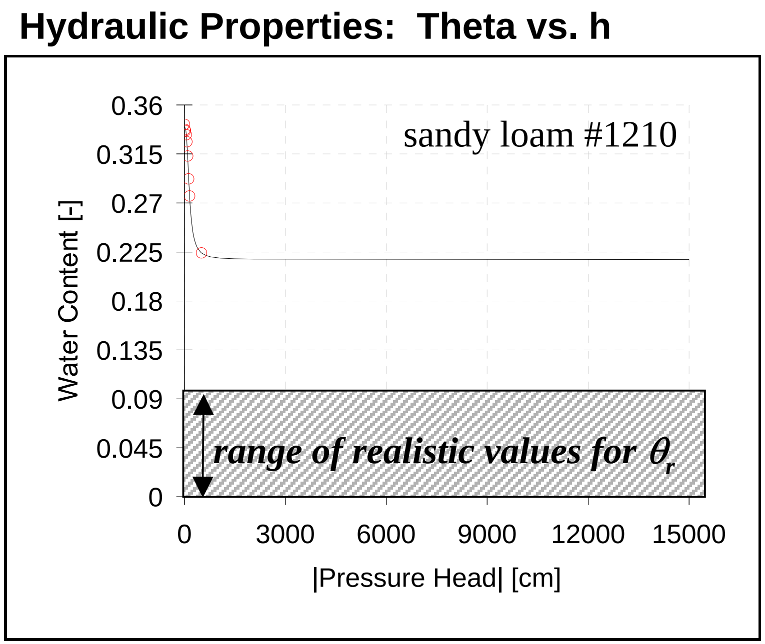
θ_r	θ_s	α	n
0.038	0.419	0.109	1.179

R^2 fitted vs obs = 0.99

Figure 2. Examples of RETC nonlinear fits of Equation 3 to experimental *θ(h)* data for 2 soils.

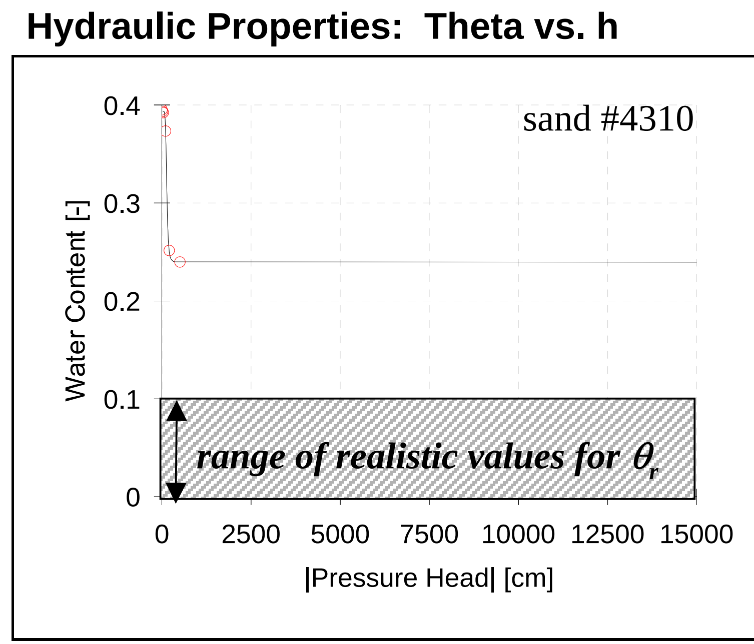
Figure 3. Cumulative distribution of minimum soil water pressure heads (h, cm) for loam, sandy loam, loamy sand and sand $\theta(h)$ data in UNSODA database. Includes a total of 321 soils.





θ_r	θ_s	α	n
0.22	0.34	0.080	3.13

R^2 fitted vs obs = 0.99

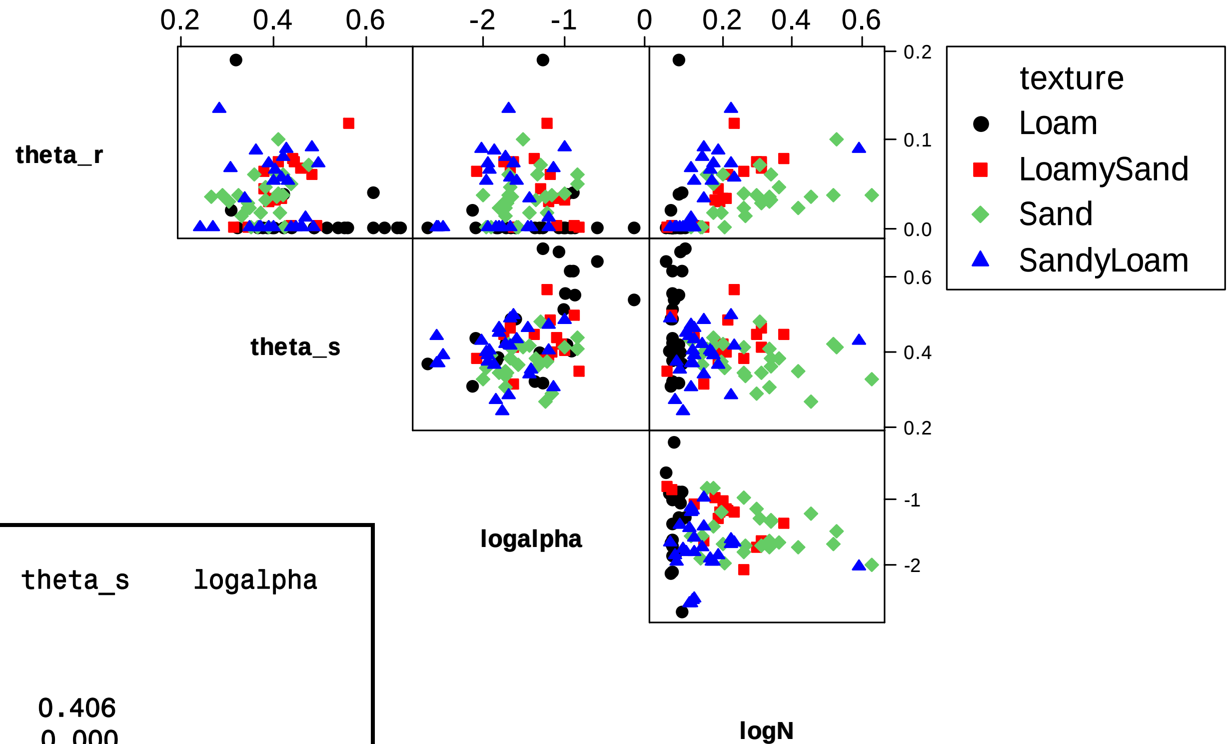


θ_r	θ_s	α	n
0.24	0.39	0.077	6.75

R^2 fitted vs obs = 1.00

Figure 4. Examples of unrealistic RETC nonlinear fits of Equation 3 to experimental $\theta(h)$ data. Note unrealistic fitted values for residual water content θ_r.

Figure 5. Matrix plot and correlation of fitted VG parameters for 90 UNSODA soils studied here.



	theta_r	theta_s	logalpha
theta_s	-0.115 0.281		
logalpha	0.041 0.700	0.406 0.000	
logN	0.448 0.000	-0.258 0.014	-0.148 0.165

Cell Contents: Pearson correlation
P-Value

Figure 6. Effect of the shape parameter *n* on soil water retention curve. Calculated using Equation 3, using parameters for soil 1290: θ_s = 0.410, θ_r = 0.065, α = 0.075

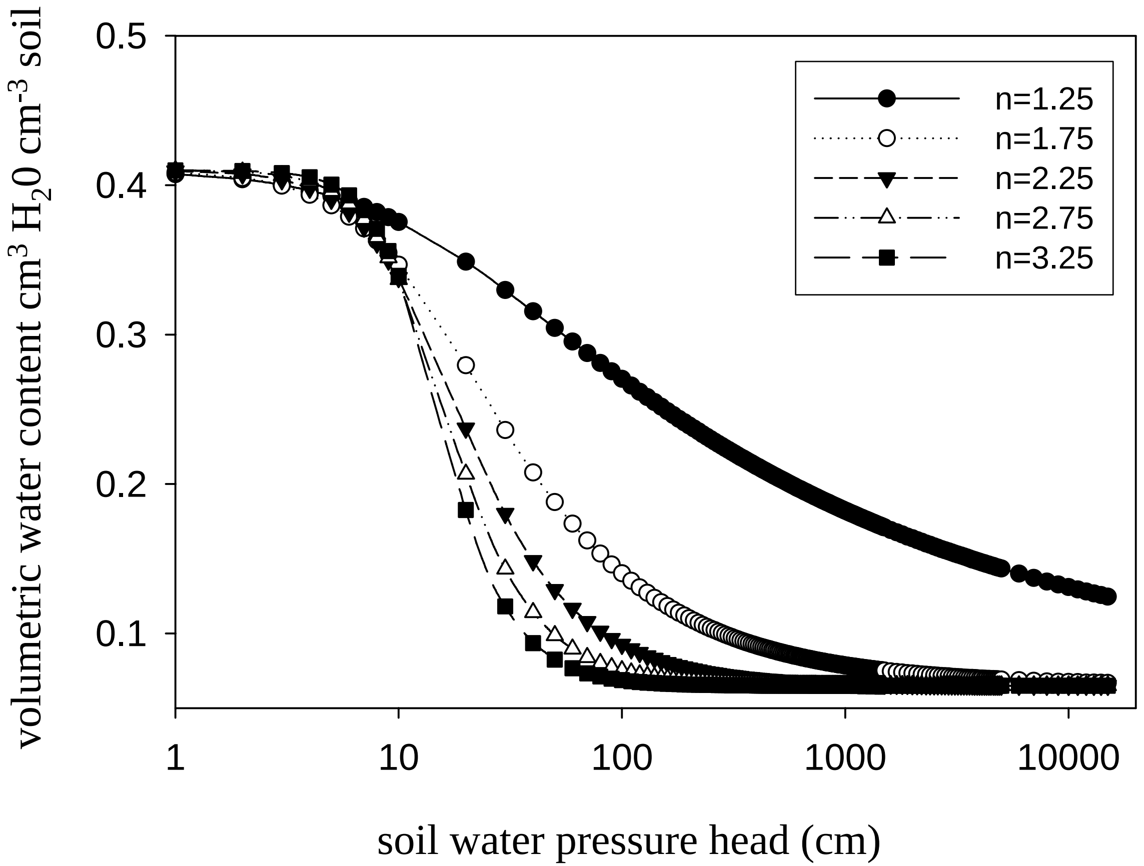


Figure 7. Soil water characteristic curves for 90 soils by soil textural class based on fitted van Genuchten parameters. Dark curve in each plot is characteristic curve calculated from PTF#1 textural class mean VG parameters.

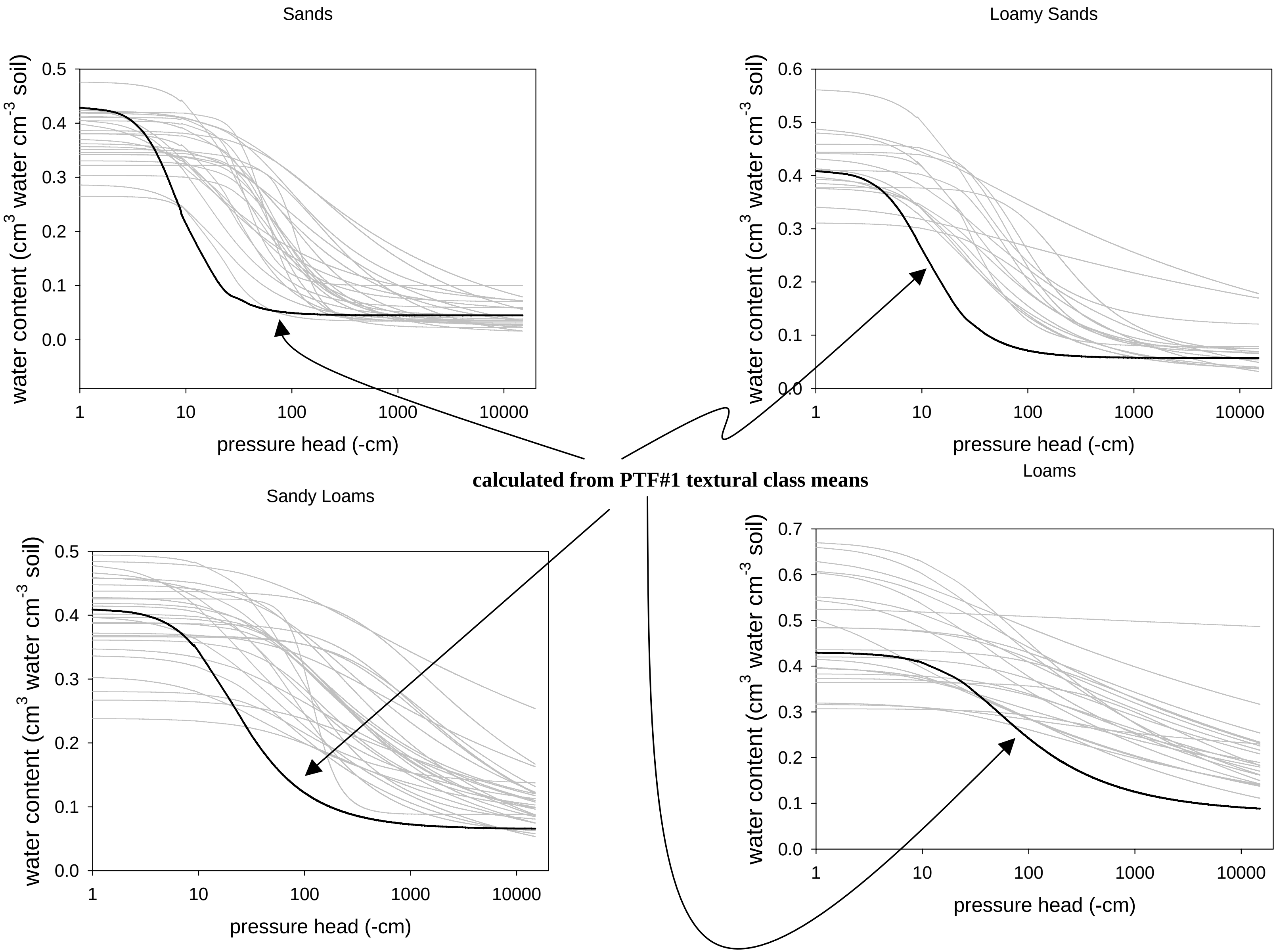


Figure 8. Predicted vs. observed water content data for 90 soils. Predicted data calculated from Equation 3 using VG parameters estimated using 6 methods: direct fitting of Equation 3 to experimental data, and PTF#1 – PTF#5. Inset numbers are correlation (top) and mean water content difference (observed-predicted; bottom).

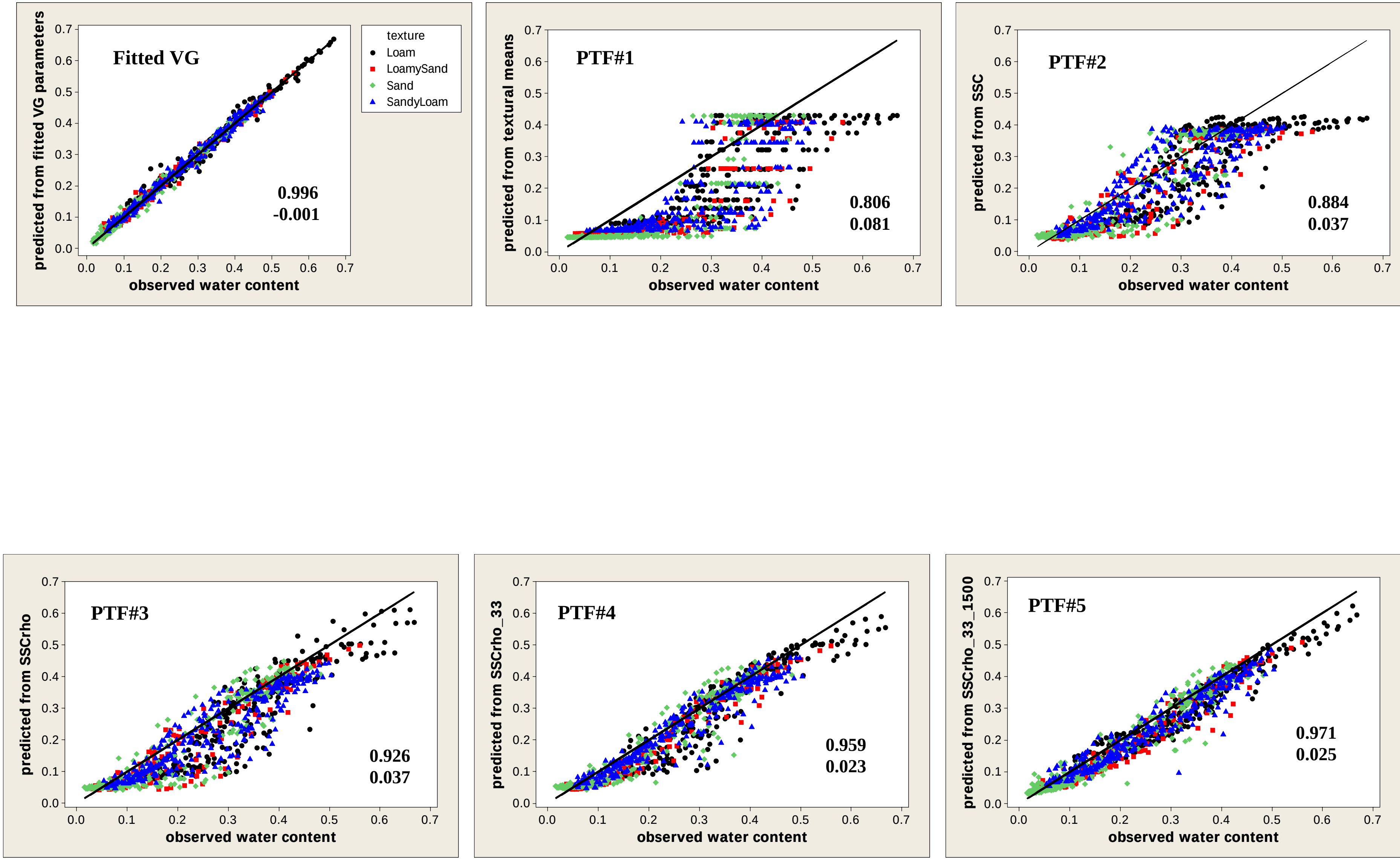


Figure 9. No tarp scenario. Box plots of simulated flux ratio by VG parameter estimation method and soil texture.

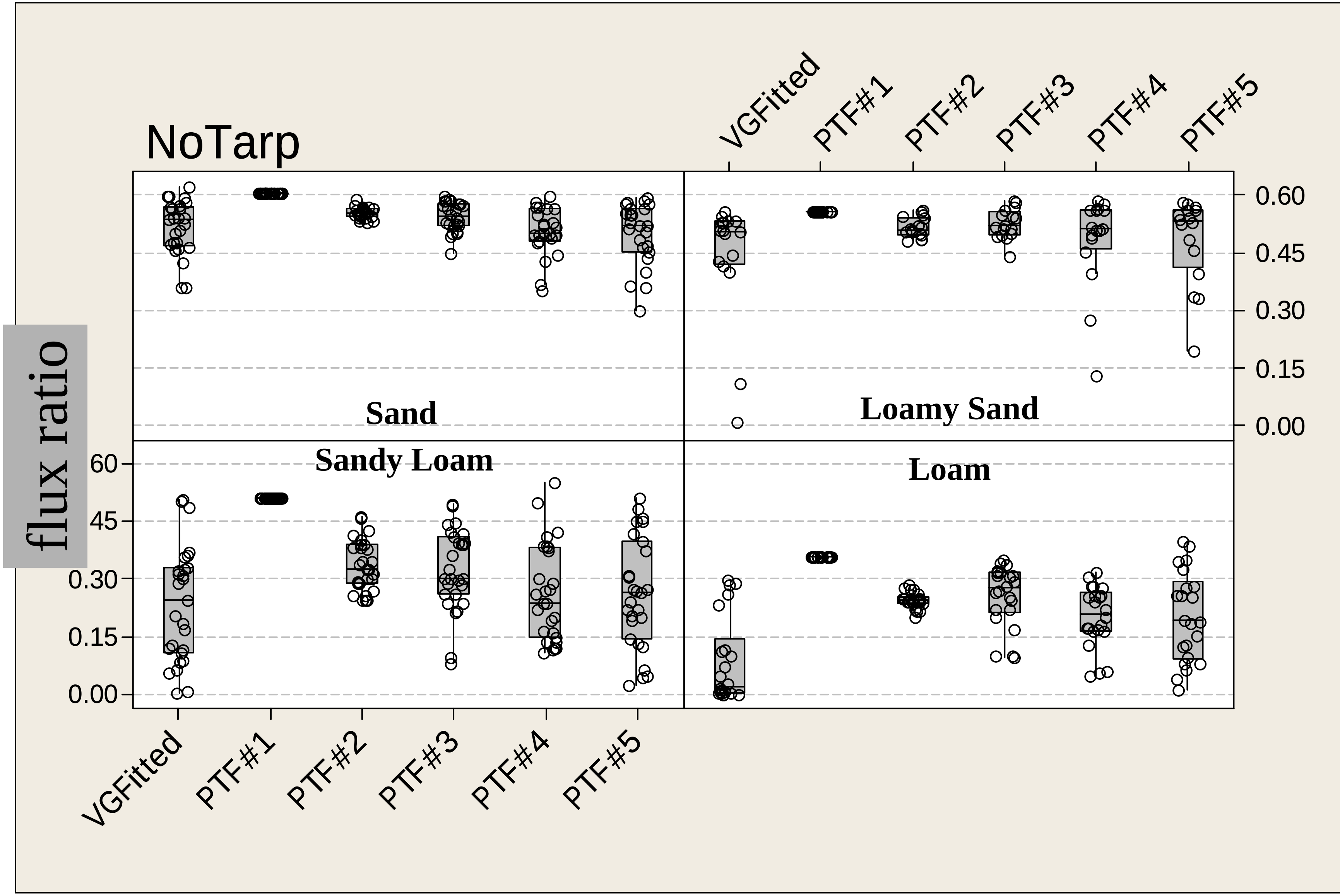


Figure 10. Tarp scenario. Box plots of simulated flux ratio by VG parameter estimation method and soil texture.

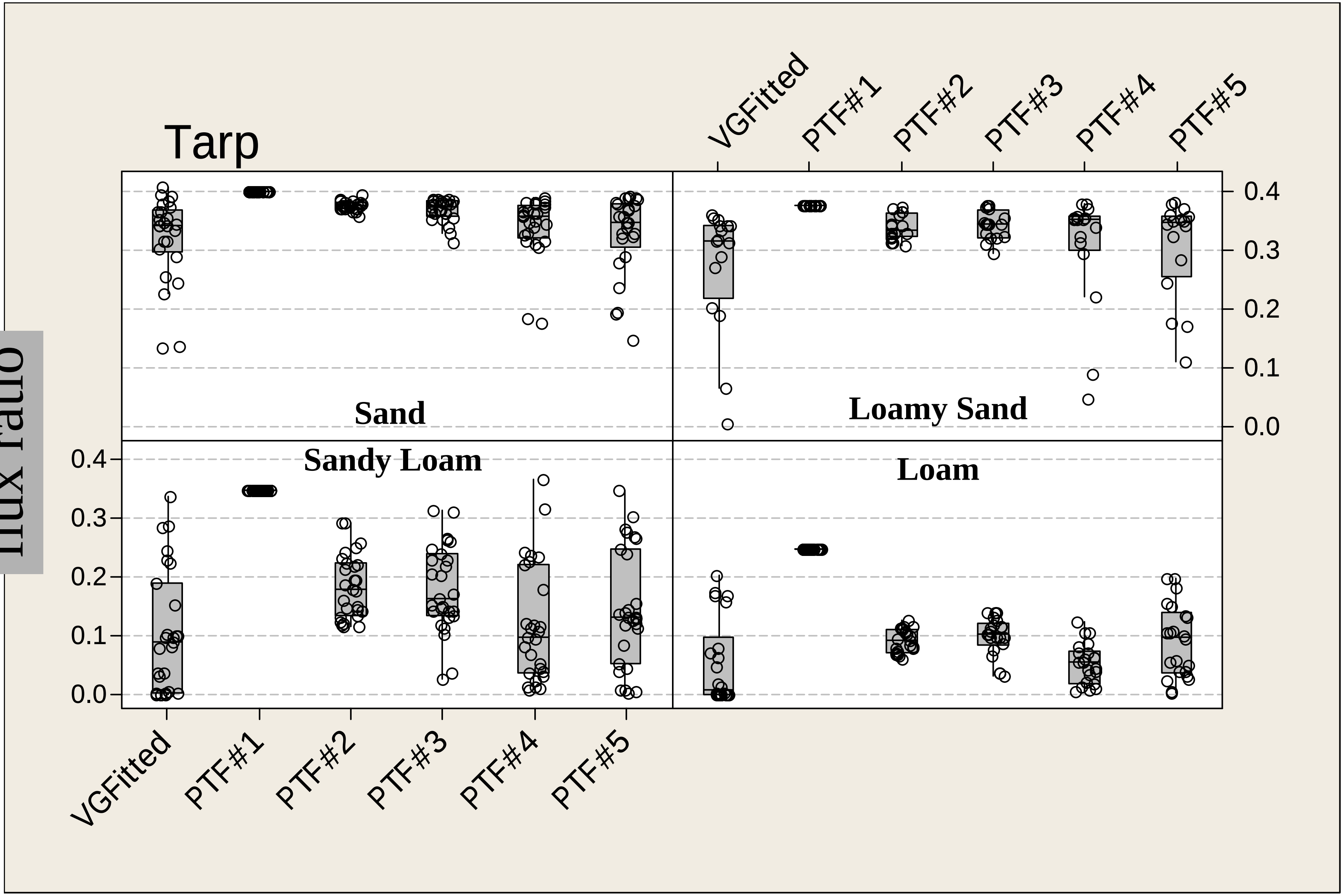


Figure 11. No tarp scenario. Box plots of Flux ratio <u>differences</u> by PTF and textural class. Differences calculated as (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$).

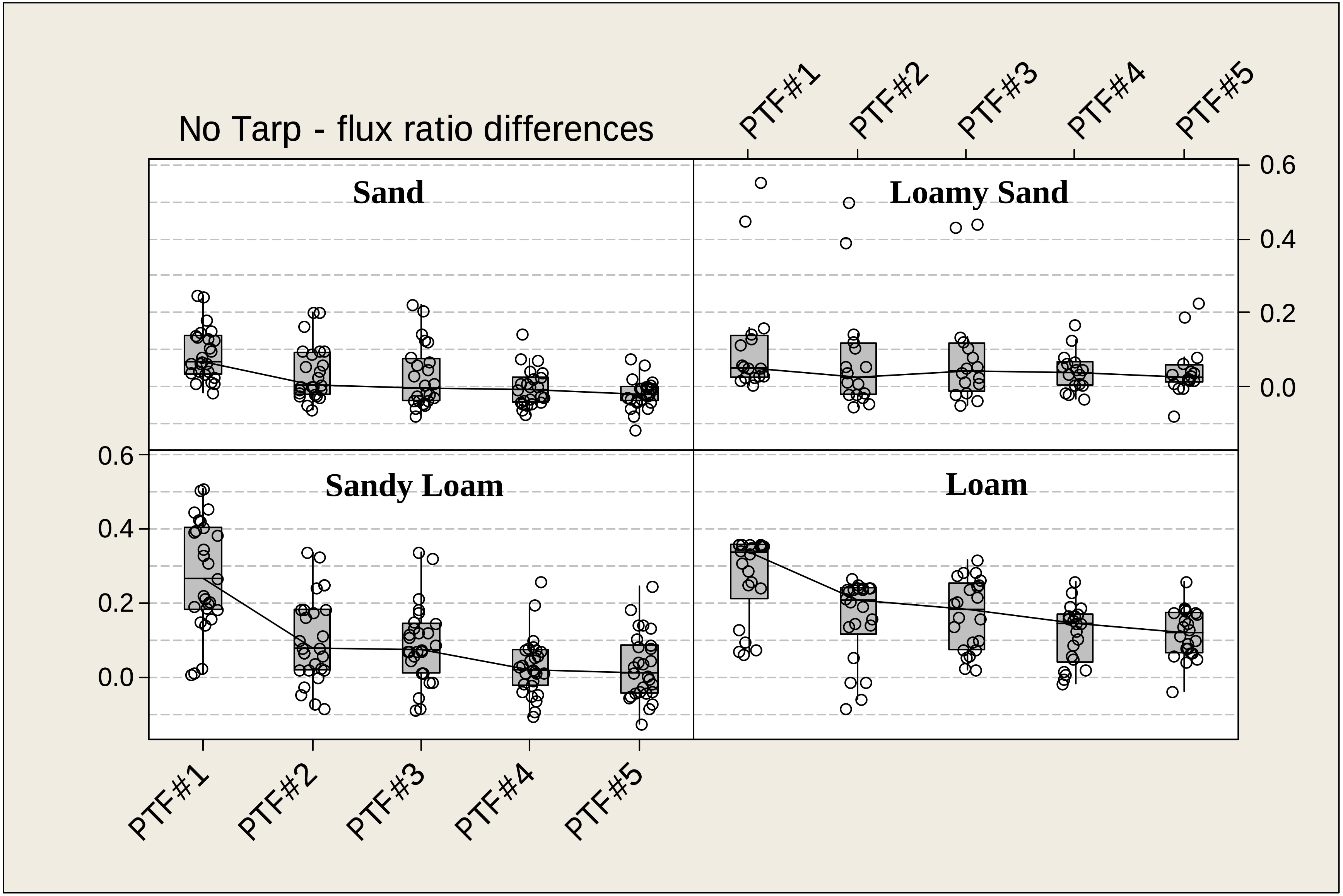


Figure 12. Tarp scenario. Box plots of Flux ratio differences by PTF and textural class. Differences calculated as (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$).

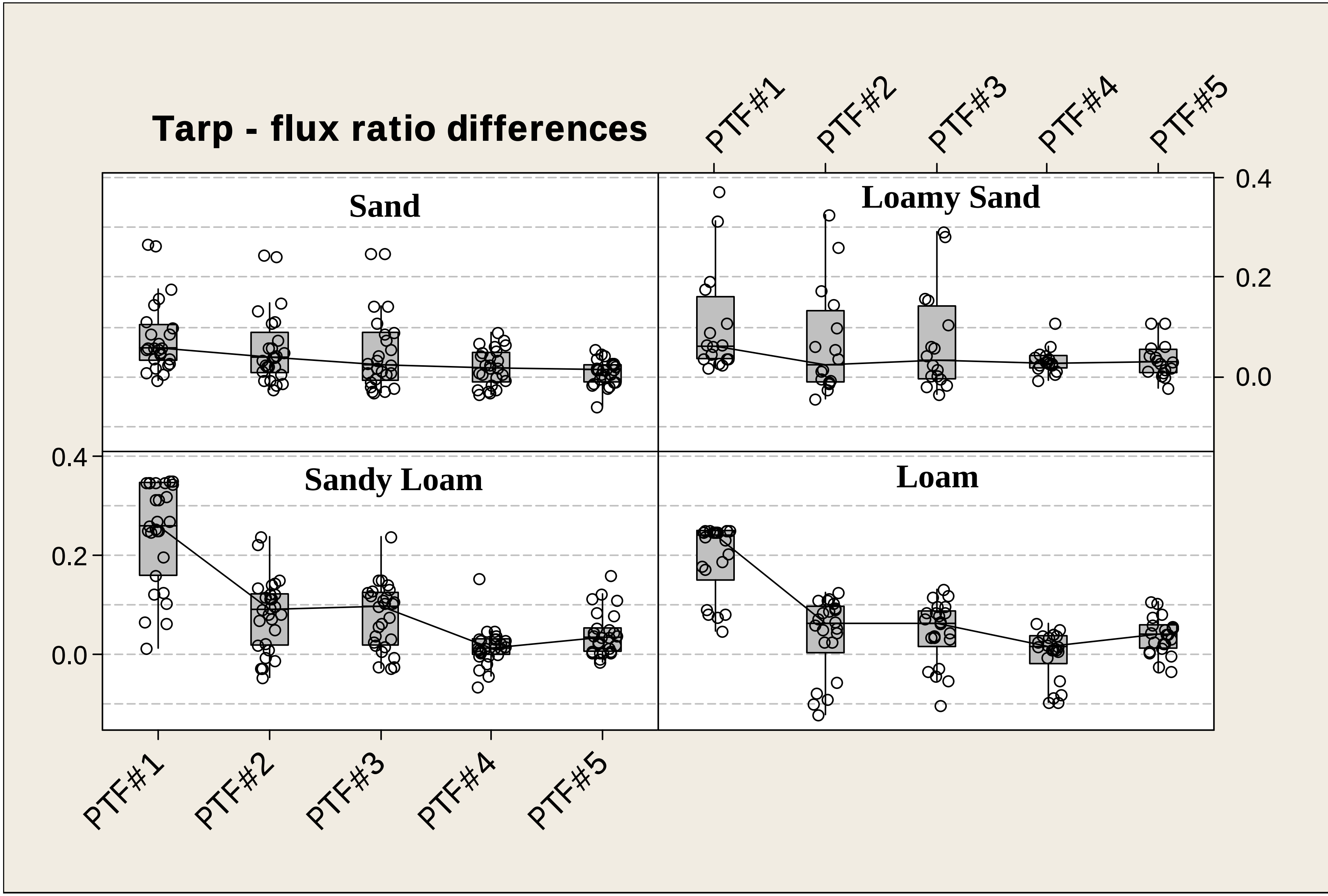
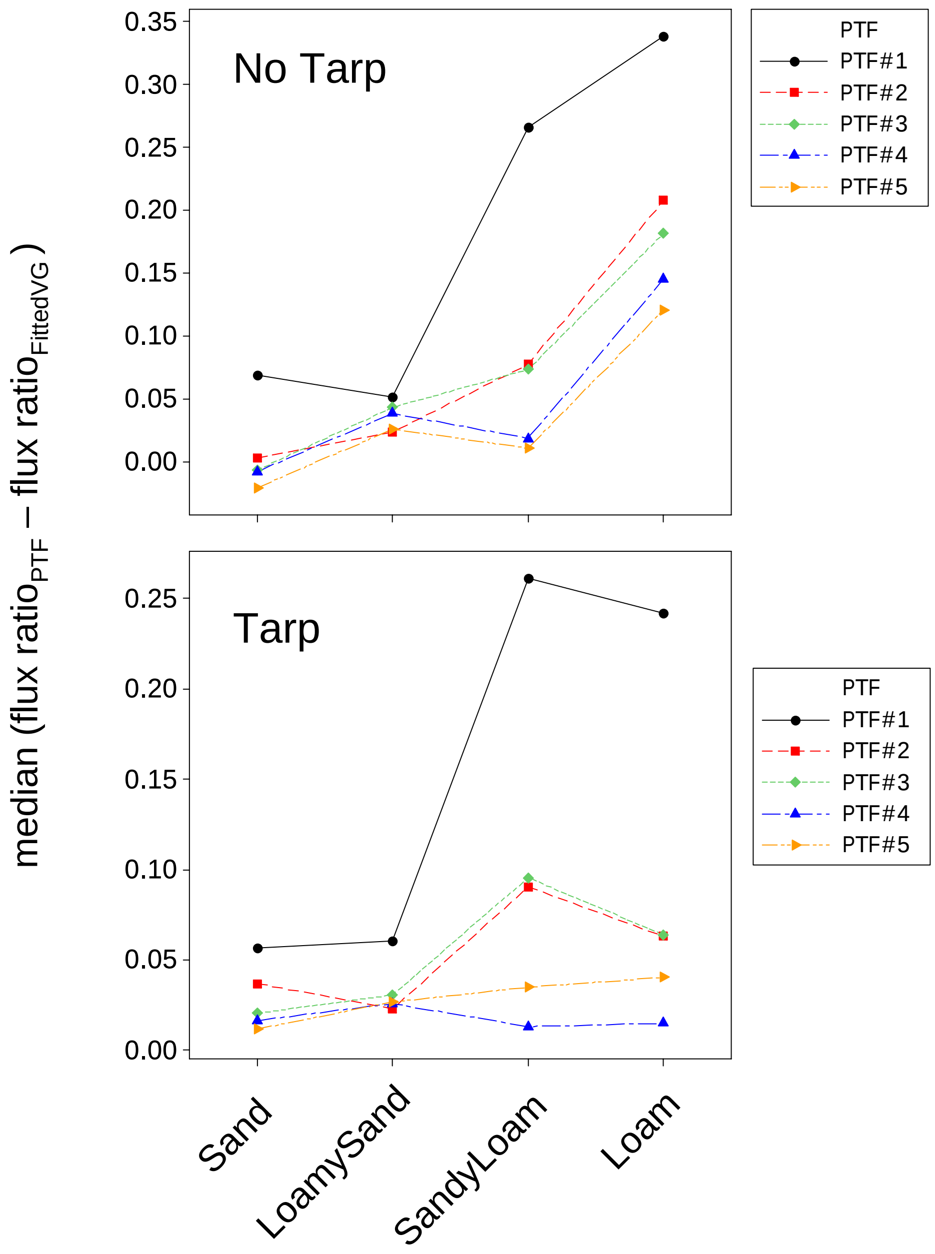


Figure 13. Interaction plot of PTF flux ratio <u>differences</u> by scenario and texture. Differences calculated as (flux ratio$_{PTF}$ – flux ratio$_{FittedVG}$).



Appendix 1

Sample input file SELECTOR.IN

```
Pcp_File_Version=4
*** BLOCK A: BASIC INFORMATION *****************************************
Heading
volatile solute - bare ground
LUnit  TUnit  MUnit  (indicated units are obligatory for all input data)
cm
days
g
lWat   lChem lTemp  lSink lRoot lShort lWDep lScreen lVariabBC lEquil lInverse
 t     t     t      f     f     t      t     t       t         t         f
lSnow  lHP1   lMeteo  lVapor  lDummy  lFluxes lDummy  lDummy  lDummy  lDummy
 f       f       f       f       f       f       f       f       f       f
NMat    NLay  CosAlpha
  1       1       1
*** BLOCK B: WATER FLOW INFORMATION ************************************
MaxIt   TolTh   TolH       (maximum number of iterations and tolerances)
  30   0.0001    0.1
TopInf WLayer KodTop InitCond
 f     f      -1       f
BotInf qGWLF FreeD SeepF KodBot DrainF  hSeep
 f     f     t     f     -1      f      0
         rTop         rBot        rRoot
           0            0            0
    hTab1   hTabN
    1e-006   10000
    Model   Hysteresis
      0          0
   thr     ths    Alfa      n         Ks       l
  0.065    0.41   0.075    1.89        500     0.5
*** BLOCK C: TIME INFORMATION ******************************************
        dt       dtMin       dtMax     DMul    DMul2  ItMin ItMax  MPL
       0.01      1e-006         0.1     1.3     0.7     3     7     2
      tInit        tMax
       0.25          21
  lPrintD  nPrintSteps tPrintInterval lEnter
     f          1             1       f
TPrint(1),TPrint(2),...,TPrint(MPL)
                 21
*** BLOCK E: HEAT TRANSPORT INFORMATION
*************************************************************
    Qn      Qo    Disper.    B1          B2          B3          Cn          Co
Cw
   0.57    0.01 4.67825e-038 1.56728e+016 2.53474e+016 9.89388e+016 1.43327e+014
1.8737e+014 3.12035e+014
      tAmpl     tPeriod    Campbell   MeltConst  lDummy  lDummy  lDummy  lDummy
lDummy
          5           1          0       0.43       f       f       f       f
f
      kTopT       TTop      kBotT       TBot
          1          20          0         20
*** BLOCK F: SOLUTE TRANSPORT INFORMATION
*****************************************************
 Epsi  lUpW  lArtD lTDep    cTolA    cTolR   MaxItC    PeCr  No.Solutes  lTort
iBacter   lFiltr  nChPar
  0.5     f     f     t         0         0     1        2        1       t
0        f       16
```

```
iNonEqul lWatDep lDualNEq lInitM  lInitEq lDummy  lDummy  lDummy  lDummy  lDummy
lDummy
   0       f       f       f       f       f       f       f       f       f
f
     Bulk.d.     DisperL.      Frac      Mobile WC (1..NMat)
        1.5          15           1           0
         DifW       DifG                n-th solute
      0.825        7125
         Ks          Nu         Beta        Henry       SnkL1       SnkS1
SnkG1       SnkL1'      SnkS1'      SnkG1'      SnkL0       SnkS0       SnkG0
Alfa
      0.187           0           1       0.066        0.05        0.05
0           0           0           0           0           0           0
0
Temperature Dependence
         DifW       DifG                n-th solute
      15000        5000
         Ks          Nu         Beta        Henry       SnkL1       SnkS1
SnkG1       SnkL1'      SnkS1'      SnkG1'      SnkL0       SnkS0       SnkG0
Alfa
          0           0           0       35000           0           0
0           0           0           0           0           0           0
0
      kTopSolute  SolTop    kBotSolute  SolBot
         -2           0           0           0
      dSurf          cAtm
        150          0
      tPulse
         21
*** END OF INPUT FILE 'SELECTOR.IN' ************************************
```

Appendix 2

Analysis of variance: soil water pressure head and texture effect on fitted log(n) and log(α)

scatterplot log(n) vs θ_r by texture

scatterplot log(n) vs minimum soil water pressure head h

scatterplot θ_r vs minimum soil water pressure head h

Appendix 2. ANOVA: testing effect of soil texture and "headrange" on fitted residual water content θ_r and log(n) using data from 321 UNSODA sands, loamy sands, sandy loams, and loams. The fitted VG parameters obtained by export from ROSETTA's MS ACCESS data base (May 2008 ROSETTA download, Table="FittedVG"). The categorical variable "headrange" refers to whether the *minimum* soil water pressure head for a soil's θ(h) data is less than –1000cm (**less_-1000cm**) or greater than –1000cm (**greater_-1000cm**).

****

General Linear Model: log_n, thetar versus headrange, texture

Factor	Type	Levels	Values
headrange	fixed	2	greater_-1000cm, less_-1000cm
texture	fixed	4	Loam, Loamy Sand, Sand, Sandy Loam

Analysis of Variance for log_n, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F	P
headrange	1	5.2287	2.2330	2.2330	103.48	**0.000**
texture	3	5.7127	5.7919	1.9306	89.46	**0.000**
headrange*texture	3	0.1313	0.1313	0.0438	2.03	0.110
Error	313	6.7544	6.7544	0.0216		
Total	320	17.8272				

S = 0.146900   R-Sq = 62.11%   R-Sq(adj) = 61.26%

Analysis of Variance for thetar, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F	P
headrange	1	0.266856	0.342417	0.342417	113.11	**0.000**
texture	3	0.067154	0.065118	0.021706	7.17	**0.000**
headrange*texture	3	0.080244	0.080244	0.026748	8.84	**0.000***
Error	313	0.947557	0.947557	0.003027		
Total	320	1.361811				

*** see interaction plot next page – effect on loam >> sand etc.**

S = 0.0550212   R-Sq = 30.42%   R-Sq(adj) = 28.86%

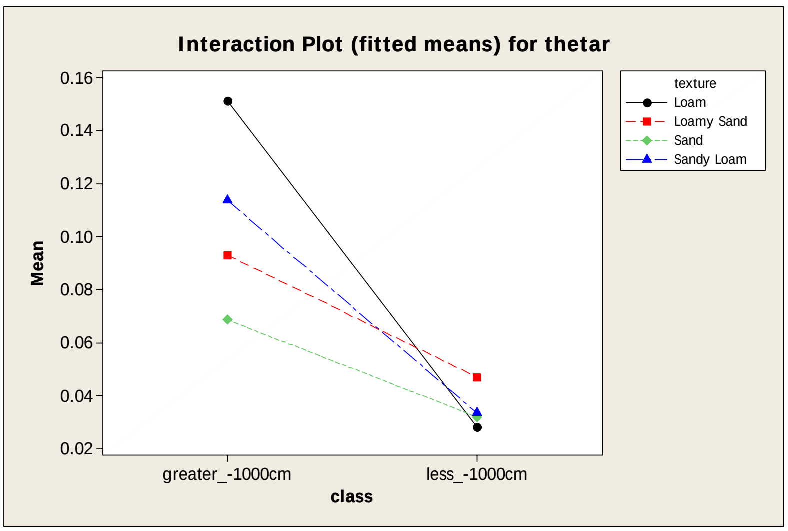
Tukey 95.0% Simultaneous Confidence Intervals
Response Variable log_n
All Pairwise Comparisons among Levels of headrange
headrange = greater_-1000cm subtracted from:

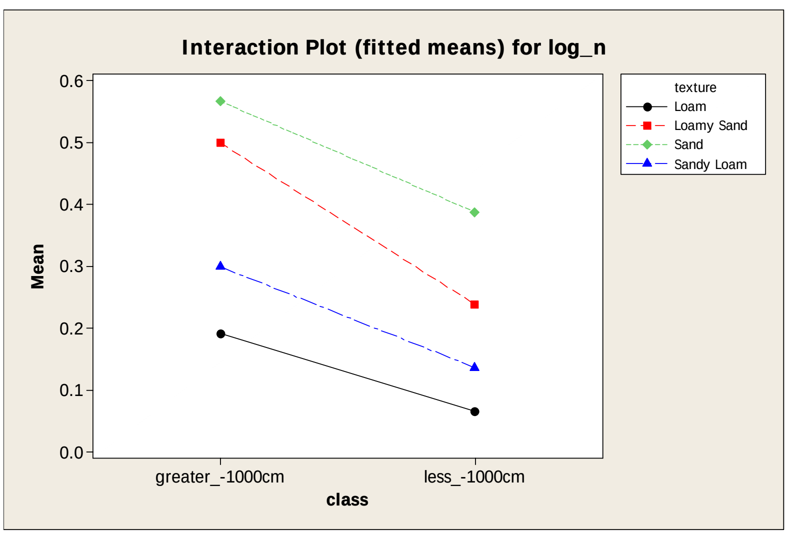
```
headrange       Lower   Center    Upper  ------+---------+---------+---------+
less_-1000cm  -0.2176  -0.1823  -0.1471  (-----*----)
                                         ------+---------+---------+---------+
                                            -0.180    -0.120    -0.060     0.000
```

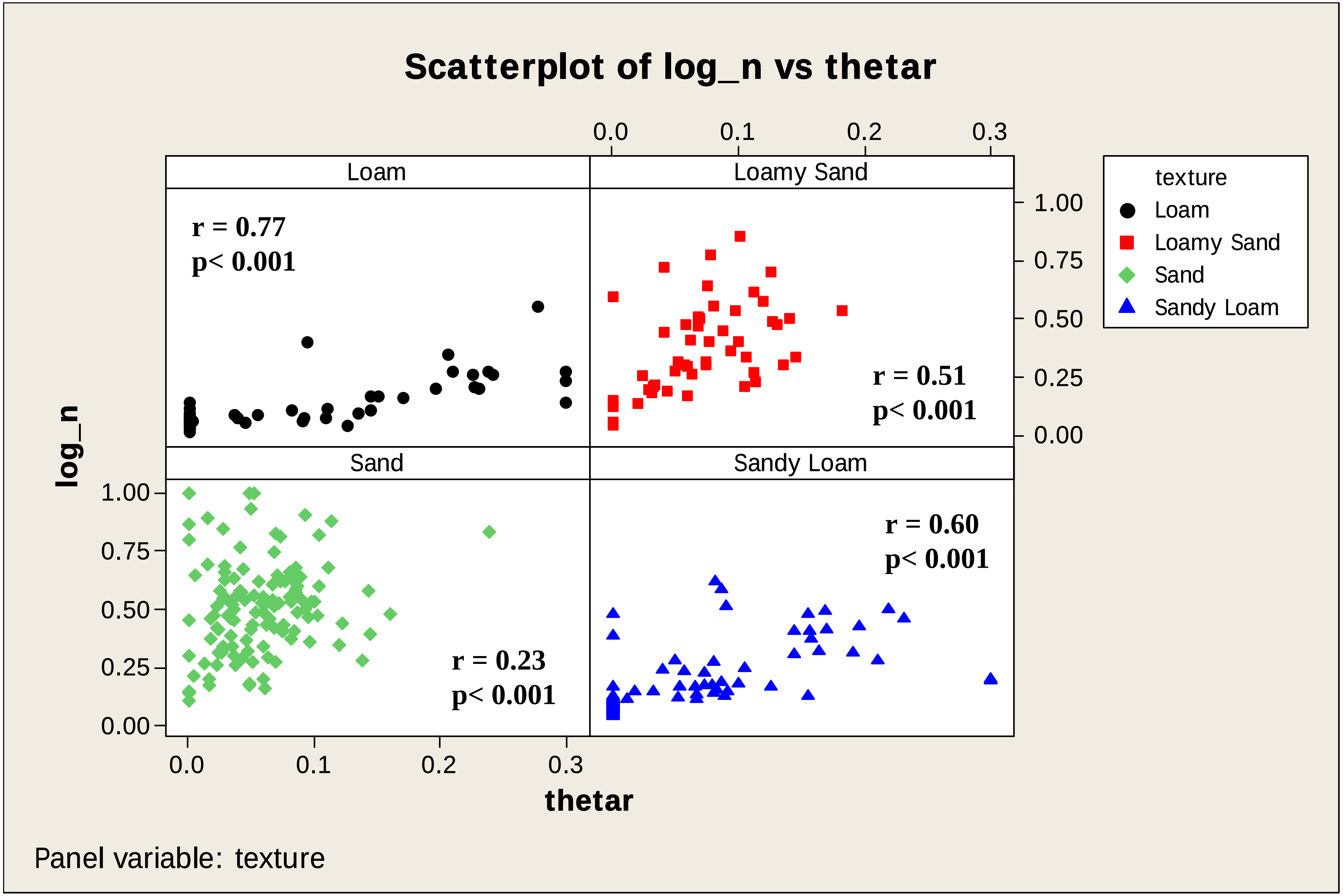
Tukey Simultaneous Tests
Response Variable log_n
All Pairwise Comparisons among Levels of headrange
headrange = greater_-1000cm subtracted from:

headrange	Difference of Means	SE of Difference	T-Value	Adjusted P-Value
less_-1000cm	-0.1823	0.01792	-10.17	**0.0000**

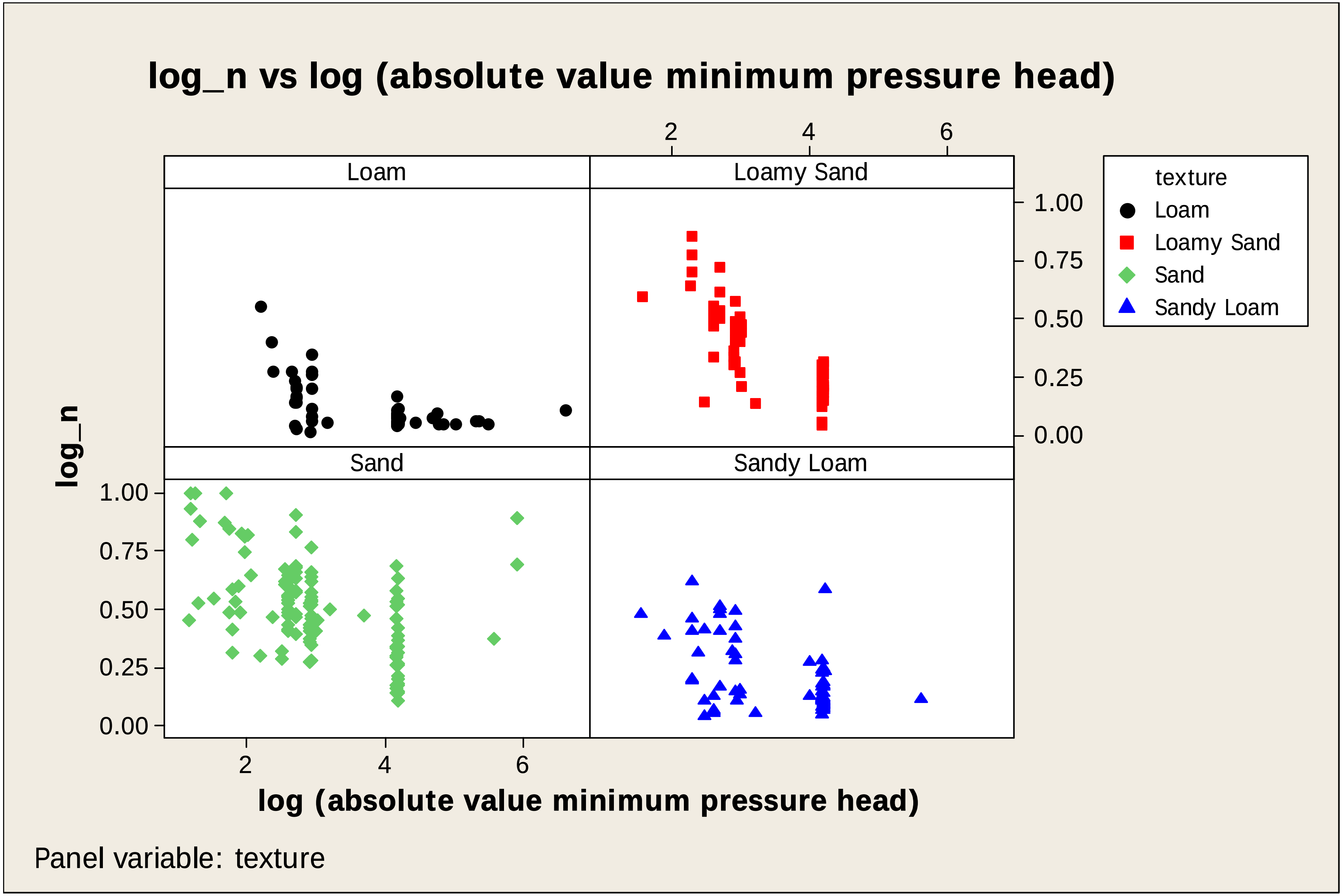
```
Tukey 95.0% Simultaneous Confidence Intervals
Response Variable thetar
All Pairwise Comparisons among Levels of headrange
headrange = greater_-1000cm  subtracted from:

headrange        Lower    Center     Upper  ----+---------+---------+---------+--
less_-1000cm  -0.08461  -0.07140  -0.05819  (----*-----)
                                            ----+---------+---------+---------+--
                                             -0.075    -0.050    -0.025    -0.000


Tukey Simultaneous Tests
Response Variable thetar
All Pairwise Comparisons among Levels of headrange
headrange = greater_-1000cm  subtracted from:

              Difference       SE of            Adjusted
headrange       of Means  Difference  T-Value    P-Value
less_-1000cm    -0.07140    0.006713   -10.64     0.0000
```



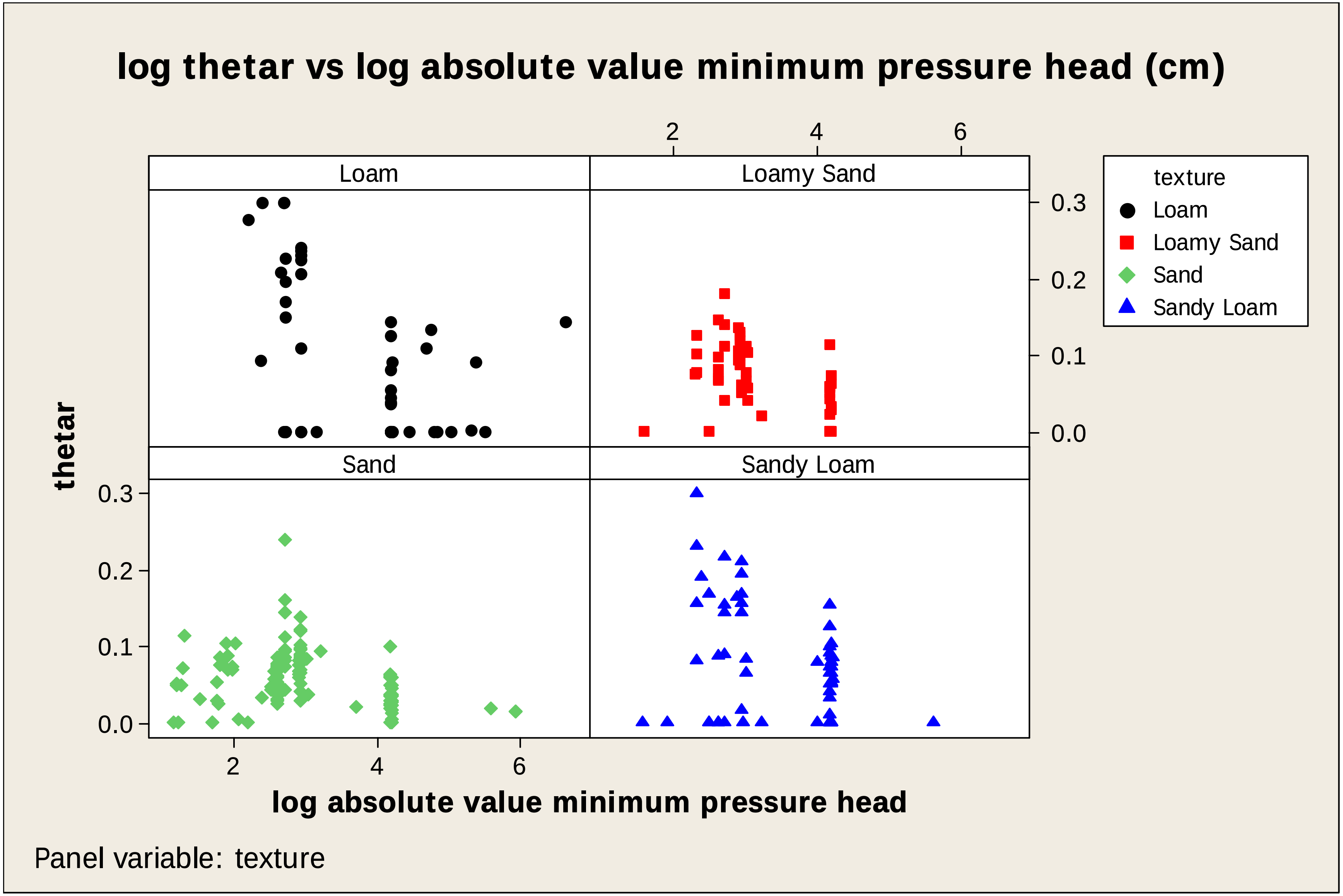




Scatterplot of log_n vs thetar
Loam
Loamy Sand
Sand
Sandy Loam
r = 0.77
p< 0.001
r = 0.51
p< 0.001
r = 0.23
p< 0.001
r = 0.60
p< 0.001
texture
Loam
Loamy Sand
Sand
Sandy Loam
log_n
thetar
0.0
0.1
0.2
0.3
0.00
0.25
0.50
0.75
1.00
Panel variable: texture



log of fitted VG parameter "n" vs. log of absolute value of minimum pressure head *h* (cm) in the soil θ(*h*) data used to obtain that fitted "n".



log of fitted residual water content vs. log of absolute value of minimum pressure head *h* (cm) in the soil θ(*h*) data used to obtain that fitted residual water content.