Statistical Optimization of Hydraulic Parameters of a Soil-Tree-Atmosphere Continuum Model of a Sierra Nevada White Fir

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Abstract

TEXT

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1. Introduction

Trees play a key role in controlling the water and energy balance at the land-air surface. As a physical medium, they transport water from the soil along a water potential gradient to the canopy, where it is transpired into the atmosphere. Thus changing water content of soil and atmosphere, they influence meteorological, climatological and hydrological cycles.

Numerical models allow simulating the relevant processes, most importantly

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the transport of water as it enters the soil, is transported through the soil, taken up by roots into the tree and ultimately transpired into the atmosphere. Early attempts to model tree water flow were often based on an analogy to an electrical circuit proposed first by Van den Honert (1948). The main motivation for drawing on this analogy is a time lag between sap flux and transpiration rate that is caused by the tree’s capacity to store water (Waring and Running, 1978; Jarvis et al., 1981), and the resistance of the xylem to water flow. Models of varying complexity have been introduced (e.g. Cowan, 1965; Tyree, 1988; Da Silva et al., 2011), but a number of problems have been identified. This approach has limitations modeling water flow since it is inadequate in separating changes in saturation change from changes in pressure (Aumann and Ford, 2002), and thus fails e.g. to consider the influence of saturation on hydraulic conductivity (Kramer and Boyer, 1995). Another problem is that the electrical circuit model allows for negative values, since electrical charges can be positive and negative. Water content, however, is strictly positive, but nothing in the model inherently prevents it from becoming negative (Chuang et al., 2006). Finally, physical flow processes in sap wood are a multi-phase flow problem, since both air and water interact in the xylem vessels (Aumann and Ford, 2002).

Attempts have been undertaken to alleviate these problems, e.g. Frueh and Kurth (1999) draw from a connection to hydrological models and treats trees as a porous medium (Siau, 1984) by considering hydraulic capacitance varying with pressure. However, more recent studies have fully given up the electric circuit analogy as advocated by Fiscus and Kaufmann (1990) and embraced physics based hydrological models (Kumagai, 2001; Aumann and
33 Ford, 2002; Bohrer et al., 2005; Chuang et al., 2006; Siqueira et al., 2008; Janott et al., 2011; Kamai et al., 2012).

34 These models discretize the modeled domain into small elements and use finite-difference or finite-element methods to solve the flow equations. Of the models presented, some concentrate on only the canopy (Bohrer et al., 2005; Chuang et al., 2006) or only the subsurface (Siqueira et al., 2008). A model considering soil, roots and tree as a continuum has been presented by Janott et al. (2011), but the tree is modeled as a simple chain of cylindrical elements. In this study, we make use of a recently developed model (Kamai et al., 2012) that describes the full continuum soil-root-tree in a finite-element model, with simulated unsaturated flow (Richards, 1931) in the soil and tree and stress functions (Feddes et al., 1978; Vrugt et al., 2001b) determining spatially distributed root uptake and canopy transpiration sink terms.

35 To fully describe the flow processes, we must parameterize water retention and unsaturated hydraulic conductivity functions (Mualem, 1976; van Genuchten, 1980). To make a model representative of nature, the parameters of these functions have to be calibrated by comparison to observational data. While parameters can also be measured e.g. in the laboratory, these measurements are mostly destructive (e.g. Heine, 1970; Zimmermann, 1978; Waring and Running, 1978; Cochard, 1992a; Sperry and Ikeda, 1997; Li et al., 2008).

36 Better understanding of the system soil-root-tree-atmosphere, however, can be gained from monitoring of hydrologic processes in soil and tree. To this end, non-destructive measurement techniques exist to resolve the temporally and spatially variable hydrologic states of the soil-tree-atmosphere system. A range of techniques allow measuring the water content of the soil,
with point probes methods like time domain reflectometry (TDR) (Noborio, 2001; Robinson et al., 2008), capacitive probes (Bogena et al., 2007; Kizito et al., 2008) and heat pulse probes (Mori et al., 2003; Kamai et al., 2009). In recent years, hydrogeophysical methods have increasingly been established that use geophysical techniques to retrieve water content distributions without disturbing the soil (see e.g. Huisman et al., 2003; Rubin and Hubbard, 2005; Vereecken et al., 2006; Rings et al., 2008). The water uptake of the tree can be monitored by sap flux sensors (..), while the water potential of the tree is retrieved from leaf water potential measurements (..).

The goal of this study was to implement an optimization framework that allows the identification of the hydraulic parameters of the tree, along with parameters of the soil and root models. Optimization can be understood as an iterative process that adjusts parameters until the smallest discrepancy is found between modeled and measured observational data. Data was collected on a White Fir in a mountaineous environment in the Sierra Nevada. There are several reasons for using a modern statistical optimization framework: (a) the large number of parameters enforces the use of a powerful method that is able to handle complexly shaped objective spaces, (b) statistical inference should be seen as a tool to learn about the model and the natural processes, e.g. by appraising model and measurement errors as uncertainty in the optimized parameters, and (c) modern computer clusters and state-of-the-art MCMC algorithms (Vrugt et al., 2008a, 2009a; Laloy and Vrugt, 2011) provide the technical opportunity to implement such a framework.
2. Site Description

The tree that is modeled in this study is a White Fir in the King’s River Experimental Watershed (KREW) in the Southern Sierra Critical Zone Observatory. Measurement operations in the observatory target a better understanding of water cycles in a changing environment, focusing on the western US mountains with its forest landscapes that are controlled by either rain or snow patterns. The measurements also focus on the interaction and feedbacks between landscape, hydrology and vegetation. In this context, Bales et al. (2011) describe a prototype instrument cluster that studies water balance on the boundary between rain and snow-dominated areas. The instrument portfolio contains central instruments like a meteorological station with eddy-covariance (flux tower) and soil water content, snow depth, matric potential and evapotranspiration monitor probes. In addition, stratified sampling captures landscape variability.

In the vicinity of the flux tower and meterological station, a White Fir (Abies concolor) tree was fully instrumented to improve understanding of the root-water-tree system in the context of the watershed experiments. The site is characterized by a shallow soil of about 2.5 m depth, underlain by saprolite and granite bedrock (...). Since the summer of 2008, more than 250 sensors were deployed to capture soil moisture content, matric potential and temperature, sap flux, stem water potential in the canopy to capture seasonal cycles of soil wetting and drying.

Figure 1 shows schematics of the site set-up with blue circles marking the six pits containing four Decagon EC5 soil moisture sensors each at depths of 15 cm, 30 cm, 60 cm and 90 cm used in this study. The tree itself is
instrumented with a heat pulse sap flow sensor (...). There is uncertainty in the amplitude of the sap flux, as the values for 2009 and 2010 differ by a factor of 3. To circumvent this problems, we introduce a sap flux amplitude scaling factor $s_{\text{sap}}$. We estimate this factor in the optimization and divide all modeled sap flux values by $s_{\text{sap}}$. This way, we still make use of the time series dynamics, which should contain a vital part of the information required to constrain the hydraulic parameters of the tree (maybe move somewhere else?).

On some dates, leaf water potential was measured by ...

We use data collected in 2009 and 2010 for two optimization scenarios. The first set encompasses 18 days starting July 15th 2009, without recorded rainfall at the end of a dry season. Sap flux was recorded every 30 minutes, soil moisture hourly and on July 21st and 22nd 2009, stem water potential was measured seven times over the course of 24 hours.

For the second data set, we use a period of 20 days starting October 2nd, since there were two major rainfall events during this period. Unfortunately, only sap flux and soil moisture measurements are available for this second data set.

3. Soil-Tree-Atmosphere Continuum Model

The flow of water is modeled as a continuum through the subdomains soil, roots and tree. We represent the model domain in a two-dimensional model that is assumed to be axisymmetrical around the center of the tree. Although the measurement pits in the soil are placed in different circle segments around the tree, this assumption allows us to include the six pits in
the two-dimensional model at their radial distance from the tree.

Atmospheric conditions force water movement, either by evapotranspiration from the soil and tree canopy into the atmosphere, or by providing rainfall that infiltrates into the soil. Figure 2 shows the setup of the model domain. The soil is divided into three layers, with the deepest layer having a low hydraulic conductivity. It models the saprolite layer between the upper soil and rock, which can store water but is not accessed by roots. The two upper soil layers have different material properties. The water taken up by roots $R_a$ is routed through a flux boundary into the second subdomain, the root buffer. The root buffer is modeled as an infinitely conductive material, so that the tree can take up the water as it needs it and the water balance is kept (Kamai et al., 2012). The third subdomain, the tree, is modeled as a rectangular domain for computational efficiency. Its size has been chosen so that the volume of the axisymmetric model tree domain is equal to that of the sapwood of the actual, conical tree.

Figure 3 gives an overview of the different water fluxes in the model. Tower data (see section 3.2) serves as the basis for obtaining the tower evapotranspiration $ET_0$ by applying the Penman-Monteith equation. This could be used as a basis for estimating bulk stomatal conductance (Baldocchi et al., 1991), however this would introduce a large number of additional unknown parameters that might not be well constrained by the available measurements. Rather, Kamai et al. (2012) have introduced a site-specific factor $s_{ET0}$ to obtain potential evapotranspiration $ET_p$ from scaling of the tower data.

We set both the potential root uptake $R_p$ and potential transpiration from
the tree $T_p$ equal to $ET_p$. The actual root uptake $R_a$ is routed into the root buffer, which the tree accesses. To remove the transpiring water $T_a$ from the tree, sink terms are placed along mesh elements in the tree domain. Section (3.3) will describe in more the model parts that determine root uptake and canopy transpiration.

3.1. Hydrological Model

To solve the equations of water flow in the model above we use an adapted version of HYDRUS (Simunek et al., 2008) that enables routing the root water uptake into the root buffer, and to model the canopy transpiration with a second Feddes model.

HYDRUS solves the Richards equation (Richards, 1931) for unsaturated water flow using a linear Galerkin approach in a finite element scheme. We assume that the parametric model by van Genuchten (1980) can describe soil water retention and hydraulic conductivity as

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} = (1 + |\alpha h^n|^{-m})^{-m}$$  \hspace{1cm} (1)

$$k(h) = k_s \sqrt{S \left[1 - (1 - S^{1/m})^m\right]^2}$$  \hspace{1cm} (2)

where $S$ is water saturation, $h$ is pressure head (cm), $\theta$ is the volumetric water content (cm$^3$/cm$^3$), $\theta_r$ is the residual water content for $h \rightarrow -\infty$, $\theta_s$ is the saturated volumetric water content, $\alpha$ is the inverse of the air-entry value (cm$^{-1}$), $n$ is an empirical shape factor (-), $m$ is a factor that can be connected to $n$ via $m=1-1/n$ and $k_s$ is the hydraulic conductivity at $\theta=\theta_s$ (cm/d).

The hydraulic parameters of the soil layers are partially determined from
laboratory measurements, but the measurement are preliminary and uncertain. Therefore, some estimation of soil hydraulic parameters has to included in the optimization. To limit the number of parameters, we restrict this to \( \log k_S \) and \( \theta_S \) of either soil layer. The other parameters are set to the laboratory values, and the deep saprolite layer keeps the parameters of the second soil layer, but with a hydraulic conductivity decreased by two orders of magnitude. ??Table with all soil hydraulic parameters??

The initial conditions are specified in terms of pressure head. For the tree, we estimate the pressure head at the base of the tree \( h_{\text{ini}, T} \) in the optimization, and then initialize the tree in hydraulic equilibrium from the base. For the soil, we first calculate the pressure head at each of the 24 soil moisture probe locations, and use a linear 2D interpolation scheme to approximate the initial distribution in between the measurement pits. The pressure heads at the left, right and bottom boundary of the area covered by probes are extended to the edges of the modeled domain, and extended with in hydraulic equilibrium above the -15 cm probe. Figure 6 shows the initial pressure head distribution for the 2009 period.

3.2. Atmospheric Boundary

For one of the two periods simulated, rainfall was measured at (...). As this was not measured under canopy, effects of rainfall interception and surface runoff are unknown. Therefore, we scale the rainfall by a parameter \( s_{\text{rain}} \) and include that parameter in the optimization.
3.3. Root and Canopy

To connect soil and tree domain of the model, water uptake by roots and transpiration has to be modeled. In the following, the root water uptake model is described, which is based on the idea of introducing a sink term at each node of the model mesh. The same idea can be used to model canopy transpiration, by introducing a sink term on the nodes of the tree domain. The distribution models the canopy shape, therefore sink terms start at 6 m and above and linearly decrease with height to the top.

3.3.1. Root Density Model

We rely on a two-dimensional root distribution model as developed by Vrugt et al. (2001a) as an extension of a one-dimensional model introduced by Raats (1974). It expresses root density as the product of a dimensionless radial distribution function ($\beta(r)$) and a depth distribution function ($\beta(z)$) as

$$
\beta(r, z) = \left(1 - \frac{z}{z_m}\right) \left(1 - \frac{r}{r_m}\right) \exp \left[- \left(\frac{p_z}{z_m} |z^* - z| + \frac{p_r}{r_m} |r^* - r| \right)\right]
$$

(3)

where $r_m$ and $z_m$ denote the maximum rooting radius and depth, $r^*$ and $z^*$ are empirical parameters that shift the maximum of the distribution in radial and depth and $p_r$ and $p_z$ are empirical factors that determine the shape of the distribution.

Two of these parameters were fixed based on knowledge acquired through the excavation of the root system of a nearby white fir stump (Eumont et al., 2012). The maximum root depth $r_m$ was set to 250 cm based on observational digs, and the maximum depth in radial direction was found by Eumont et al. (2012) to be 160 cm. The other parameters were added to the optimization.
It could be expected that the maximum radial rooting distance coincides with the extent of the modeling domain, however this is not clear from observations. Therefore, also $z_m$ was obtained through optimization. The resulting optimized root density distribution for the 2009 period is shown in Fig. 4.

3.3.2. Root Water Extraction

The model extracts water from the soil using a sink term that represents extraction of water from the soil by roots. In the finite element geometry, each node is assigned a sink term. The shape of the sink terms determines the proportion of potential root water uptake $R_p$ actually extracted depending on the pressure at each node as:

$$R_a(h, r, z) = \alpha(h)\beta(r, z)R_p$$

The shape of this water stress response function $\alpha(h)$ as introduced by Feddes et al. (1978) is shown in Fig. 5 and is characterized by four characteristic pressure values $P_1 \ldots P_4$.

4. Optimization Framework

As seen in the previous sections, we have to deal with (a) a large number of unknown parameters, (b) three different measurement types that all should be included in the optimization process, and (c) a desire to not only find one discrete set of parameters, but to learn about the uncertainty in the parameters.

To elaborate on the last point, there are various sources of uncertainty in
modeling a natural system, notably structural errors caused by simplifications in the way the model approaches the true processes, and errors in measuring the forcing and observations. Structural errors typically are considerably larger than modeling errors (Vrugt et al., 2009b), yet they are very hard to quantify, and the task of separating different sources of errors is a daunting one (see e.g. Keating et al., 2010, and references therein). However, it should be clear that an optimization framework that recognizes uncertainty at least implicitly, through precipitation into parameter uncertainty, provides more information than a deterministic framework that seeks only an optimal parameter set. The question whether a formal or informal framework should be used has been contested (Vrugt et al., 2009b; Beven, 2008; Vrugt et al., 2008b), but (a) a formal statistical optimization framework that is used in a way that merges all uncertainty into parameter uncertainty is used in a rather informal way and (b) it still offers the possibility of extending or using it to disentangling sources of error.

Furthermore, as we are dealing with a larger number of parameters and complex, non-linear relations between them, the objective function we seek to minimize will have a very complex shape. If we tried to use classical minimization techniques like gradient descent, there is a remarkable chance to get stuck in a local minimum. Did we try different starting positions, we would be overwhelmed by the dimensionality of the problem; if we applied regularization we would artificially cut out parameters with lower sensitivity instead of learning about their uncertainty.

Consequently, we are looking for a global optimization framework that recognizes model and measurement error implicitly or, if available, even explicitly.
Markov Chain Monte Carlo (MCMC) methods provide such a framework, and here we rely on the current state-of-the-art member of the DiffeRential Evolution Adaptive Metropolis (DREAM) family of algorithms (Vrugt et al., 2008a, 2009a, 2011; Laloy and Vrugt, 2011).

4.1. (MT)DREAM\textsubscript{ZS}

We try to understand the workings of MCMC methods from the objective of each optimization: To find the best possible agreement between a series of \( N \) observations \( Y = Y_1 \ldots Y_N \) and \( N \) modeled values \( y = y_1 \ldots y_N \) (the added complication of different observation types will be discussed later). Most often, the discrepancy between modeled and measured values is described by the sum of squares or some variant thereof:

\[
\text{SS} = \sum_{n=1}^{N} (y_i - Y_i)^2
\]  

(5)

The \( y \) are produced by a model that calculates the time development of the observed states dependent upon a set of parameters \( \theta \). By iteratively changing the parameters, we modify the modeled values and can minimize Eq. 5 if we discover good set of parameters.

MCMC methods guide Markov chains on a random walk through the parameters space. Candidate positions for a chain to jump from position \( \theta_{t-1} \) to a new position \( \tilde{\theta}_t \) are drawn from a proposal distribution \( q(\cdot) \) and accepted based with the Metropolis acceptance probability

\[
\kappa(\theta_{t-1}, \tilde{\theta}_t) = \begin{cases} 
\min \left( \frac{\pi(\theta_{t-1})}{\pi(\tilde{\theta}_t)} \right), & \text{if } \pi(\tilde{\theta}_t) > 0 \\
1, & \text{if } \pi(\tilde{\theta}_t) = 0
\end{cases} 
\]

(6)
where $\pi(\cdot)$ stands for the likelihood of a parameter set, which increases
with decreasing Eq. 5. The candidate position is always accepted as $\theta_t$ if
it has a higher likelihood, otherwise there still is a chance of moving there
(otherwise, $\theta_t = \theta_{t-1}$). This has at least two consequences: (a) the chain
can move out of local minima by chance and more importantly, (b) under
certain requirements for the proposal, the chains will converge and sample
only from a unique stationary distribution. This distribution is equal to the
posterior distribution of the parameters, containing our uncertain knowledge
about the optimal parameter region.

The key point in designing an MCMC algorithm is choosing the proposal
distribution $q(\theta_{t-1}, \cdot)$. Careless choice of the proposal will lead to slower con-
vergence, which in our case of physical hydrological models translates into
excessive computational demand. A major inefficiency in simple proposals is
that they lack recognition of scale and orientation of the stationary distribu-
tion. To this end, DREAM runs multiple Markov chains in parallel. Apart
from the benefits for calculating convergence statistics (e.g. Gelman and Ru-
bin, 1992), dealing with multimodal distributions or long-tailed distributions
(see e.g. Laloy and Vrugt, 2011, and references therein), this allows for an
elegant way of creating proposals that self-adjust to the scale and orientation
of the target distribution (ter Braak, 2006): Jumps in each chain are gener-
at from the vector connecting two other chains.

Formally, a candidate position for a jump in chain $i$ is found as

$$\tilde{\theta}^i_t = \theta^i_{t-1} + \gamma (\theta^j_{t-1} - \theta^k_{t-1}) + \epsilon$$

where $i \neq j \neq k$ (7)

with an ergodicity term $\epsilon$ that is drawn from a symmetric distribution with
variance small compared to the posterior distribution, and allows for some
random parameter space investigation. This proposal can be combined with
a self-adaptive randomized subspace sampling method to achieve a MCMC
algorithm with desirable theoretical properties of maintaining detailed bal-
ance and ergodicity (ter Braak and Vrugt, 2008; Vrugt et al., 2008a, 2009a).
This principle is demonstrated on Fig. 7, which shows a slice through the
parameter space for two parameters of the model in the optimization of the
2009 period. A larger (or less negative) objective function, corresponding to
the blue areas, is the posterior region. Two chains are shown at uniformly
sampled positions of their evolution in parameter space. The first jumps
(marked by the thick arrow) were still rather random, but then it is clearly
visible that the jumps orient their direction and scale towards the region of
higher likelihood, and end up sampling just from that region, the posterior
distribution.

Three modifications have been proposed that lead to the current variant
(MT)DREAM_{ZS}. First, the ZS stands for sampling from an archive of past
states. Sampling only from the current positions of chains as in the original
DREAM requires at least $d/2$ to $d$ chains, where $d$ is the number of pa-
rameters. This becomes very inefficient for problems with many parameters.
Therefore, Vrugt et al. (2011) proposed keeping an archive of past states to
generate candidate points. The resulting DREAM_{ZS} needs only $d = 3\ldots5$
chains and requires less function evaluations to converge.

A second modification is the introduction of Snooker updates to increase
proposal diversity (ter Braak and Vrugt, 2008), where the difference vector
in Eq. 7 is projected unto a line connecting the current chain position to
another chain.
The third addition is a multi-try algorithm implemented by Laloy and Vrugt (2011) that incorporates a multiple-try Metropolis method (Liu et al., 2000) into DREAM that tests multiple candidate points mixing small and large jumps simultaneously. Candidate points are then selected with probability proportional to their likelihood and accepted with a Metropolis ratio. This approach leads to higher acceptance of candidate points and faster convergence.

4.2. Implementation

To take advantage of the potential of running in parallel multiple chains, and within each chain, multiple tries, (MT)DREAM\textsubscript{ZS} is implemented to run on a computing cluster, running in our variant 3 chains in parallel, and 3 candidate points are created simultaneously for each chain. Snooker updates are chosen over the DREAM parallel update with a probability of 10%.

The build the objective function that measures the distance \( SS \) between modeled and measured values and is minimized by the optimization, we need to add the different measurement types in a way that gives equal weight to each series. To be able to compare all soil water measurements in one series, we calculate stored water volume by multiplying each soil moisture probe’s value with the volume it represents and restrict the calculation to a depth of 90 cm. In calculating the error between measured and modeled storage, we take each volume’s difference first and then sum, to keep the local information intact, so we obtain

\[
SS_{\text{Store}} = \sum_{n=1}^{N} \sum_{v=1}^{V} (y_{i,\text{store},v} - Y_{i,\text{store},v})^2
\]  

(8)
where the second sum runs over all volume elements $1 \ldots V$.

We weigh the individual measurement types by the number of measurements and the measurement errors, resulting in objective function for the 2009 series:

$$O_{09} = \frac{SS_{Stem}}{\sigma_{err,Stem}^2} + \frac{n_{Sap}}{n_{Stem}} \cdot \frac{SS_{Sap}}{\sigma_{err,Sap}^2} + \frac{n_{Store}}{n_{Stem}} \cdot \frac{SS_{Store}}{\sigma_{err,Store}^2}$$  \hspace{1cm} (9)

where the measurement errors $\sigma_{err}$ are heuristically set to 20% of the standard deviation of each respective measurement series, and $n_{Stem}$, $n_{Sap}$ and $n_{Storage}$ and the number of measurements in the stem water potential, sap flux and storage time series.

For the 2010 period, we have no stem water potential measurements available, therefore the above equation reduced to

$$O_{10} = \frac{SS_{Sap}}{\sigma_{err,Sap}^2} + \frac{n_{Sap}}{n_{Store}} \cdot \frac{SS_{Store}}{\sigma_{err,Store}^2}$$  \hspace{1cm} (10)

5. Results and Discussion

All the optimized parameters and their uncertainty are listed in Tables 1 and 2 with the range of the uniform prior distribution and the 95% and 50% confidence intervals along with the medians in the posterior distribution. To help assess how much the parameters were constrained and if the same parameter ranges were found for the two different optimization scenarios, Fig. 8 shows a caterpillar plot of the parameters. The rainfall scaling parameter $s_{rain}$ has been omitted since it was only optimized for the 2010 scenario. The figure shows the prior ranges in each parameter scaled to the interval between 0 and 1. The orange bars are for 2009, and are in each case immediately followed by an orange bar for the same parameter in the 2010
scenario. The width of the narrow bar indicates the 95% confidence interval of the posterior, the thick part the 50% confidence interval; and the whisker marks the median.

((TODO: Discuss how much ranges were constrained, which parameters were not identified well and where the optimizations disagree. Needs better convergence.)) A lot of the parameters agree within the margin of error, but some of the parameters were found differently for the scenarios. Among these are $\alpha$ and $n$ of the tree and the hydraulic conductivities of the soil. The values for $s_{\text{sap}}$ are expected to be different, since they compensate for different sap flux amplitudes.

5.1. Soil Water Characteristics

We compare the optimized hydraulic parameters of the tree to data reported in the literature. A brief description of the literature included is presented in appendix 7.1. Most studies are concerned in establishing a relation between relative hydraulic conductivity and water potential (or applied pressure), a so-called vulnerability curve. To facilitate comparison to these data, we use the optimized parameters to connect pressurehead and relative conductivity. To acknowledge the parameter uncertainty contained in the parameter posterior distributions that were determined by (MT)DREAMZS, we apply a bootstrap method by randomly drawing parameter combinations from the posterior distribution and displaying the area enclosing 95% of the resulting vulnerability curves. The resulting curves are found in Figures 10 and 11.

Again, due to the much narrower bounds on the 2010 optimization, the uncertainty band is very narrow as well, but is mostly in agreement within the
2009 band uncertainty. The relative conductivity for the optimized parameters generally decreases at lower pressures than in the curves reported in the literature. There is, however, good agreement to the data by Waring and Running (1978), but Domec and Gartner (2001) note that their method of cutting small flat discs of wood cuts open tracheids and leads to measurements neglecting the tension within the xylem stream, thus overestimating water capacitance, leading to underestimation of relative conductivity. Discrepancies, however, may also stem from the fact that the literature studies are conducted on branches or wood pieces only, and that we rather estimate effective hydraulic parameters for the complete tree evidence.

A second reason for the discrepancy might stem from correlation to other parameters, like the scaling parameters $s_{\text{sap}}$, $s_{\text{ET0}}$ or soil hydraulic parameters. To test for possible influence through correlation to other parameters, we check the correlation matrix of the posterior distribution. We use the recently developed distance correlation (Szekely et al., 2007; Szekely and Rizzo, 2009), which is a new measure of dependence between random vectors. It has the desirable property of being 0 only if both vectors are independent and was found to perform excellent across a range of applications. Figure 12 shows the correlation between the tree hydraulic properties and all parameters in the optimization for 2009.

Strong correlations are found between $n$ and $\alpha$. A strong correlation between these parameters has been described before (see e.g. Huisman et al., 2010), and could plausibly be cause for some uncertainty about the relative conductivity (as it determines the curve shape??). The strongest correlation, however, is found between the saturated hydraulic conductivity and the
sapflux scaling factor. Since this factor only had to be included to account for uncertainty in quantifying the amplitude of sapflux, future studies with improved sapflux measurements should find different vulnerability curves if this correlation introduced an error into the optimization. Some data were also available on the soil water characteristics, and presented with the optimized retention curves in Figures 13 and 14, again with the 95% confidence area of the optimized parameters. Here, we find good agreement within the uncertainty bounds both with the Waring and Running (1978) and Yoder (1984) studies for both years, although the 2010 uncertainty bounds again are much narrower.

5.2. Modeled vs. measured data

To evaluate how good the best set of parameters describes the measured data, we compare measured and modeled data in Figs. 15 and 16. For 2009, the potential evapotranspiration ET0 as determined from the flux tower measurements is shown in the top panel, and the site-specific potential evapotranspiration \( ET_p \) as scaled with the parameter \( s_{ET0} \) in green. The three different measurement types are shown in the next panels. A very good agreement can be found for all of the three measurement series.

The modeled sap flux can not completely capture the highest amplitudes at noon. However, as the dynamics of the time series are captured very well, and as the amplitude of the sap flux is scaled by the parameter \( s_{tap} \) we must conclude that the optimization was not able to find a better find of the dynamics with scaling leading to higher amplitudes. This, on the one hand, is encouraging since it vindicates our assumption that introducing scaling on
the sap flux would be justifiable since catching the dynamics was the primary objective. On the other hand, this also indicates that there is some error in the model setup that does not allow for even better sap flux dynamics. This might be connected to the forcing and the scaling to the site, or to structural model error through simplification, e.g. the assumption of axial symmetry.

An additional test was undertaken to check if the choice of sap flux scaling might have been influential. We chose a scaling model that included an additional intercept parameter, however this did not lead to a better fit of the amplitudes.

The stem water potential measurements are all captured very well by their model counterparts, except one very low measurement that was taken around 3 pm. This one exception might be connected to microconditions, like the branch getting more sunlight during this time and thus not being completely representative of the tree, it might also be connected to the same issues that lead the model to not fit the highest amplitudes in the sap flux quite right, or to the heterogeneities in the actual tree that are locally not captured by the effective hydraulic parameter we obtain from our optimization. To check for an effect of the measurement series weighting, we investigated a variant of the optimization with even larger weight on the stem water potential measurements. This lead to only marginally better modeling of the stem water potential, but considerably larger discrepancies in the two other modeled data types. It will remain for future investigation whether a series with stem water potential measurements over a larger time period would improve the optimization even further.

Finally, the modeled storage shows very good agreement with the measured
values, only somewhat overestimating the remaining water content in the last five days. This could be connected to the simple two layer model of the soil or to the root density distribution.

5.2.1. 2010 Period

For the second optimization scenario, the 2010 rainfall period, no stem water potential measurements were available. Figure 16 shows the evapotranspiration, the measured and scaled rainfall, and the sap flux and storage time series. While the storage again is modeled well, there are larger discrepancies between modeled and measured sap flux, most prominently the amplitudes are severely underestimated.

There could be a number of factors contributing. First, it is visible that the measured time series is of more questionable quality. We already mentioned that differences in amplitude compared to 2009 as motivation to introduce the scaling factor $s_{\text{sap}}$. But the time series also contains a baseline value it doesn’t fall below, and that wasn’t present in the 2009 series. It is not very plausible that the tree actually kept a constant flux value during the night time under changing environmental conditions. This rather could be instrument degradation, as it is a well known effect in sap flux probes that the tree regrows around the wound inflicted by the probe installation and possibly cuts off the probe from sap flow paths. This would also explain the overall lower amplitudes in 2010 compared to 2009, however this is not completely clear at this point. This baseline can not be captured by the model and throws off the optimization. Additionally, spurious sap flux measurement can be seen on day 277 and 278. These however do not seem to have
any impact on the quality of the optimization. In addressing the baseline problem, experiments with a two parameter sap flux scaling with intercept as described above did not lead to a better fit. Future measurements in the project with newly installed sap flux sensors will provide better information about the complexities of the sap flux measurements and hopefully improve the optimization results.

A second reason might be the spatial separation of rainfall measurements and tree. We somewhat addressed this with a rainfall scaling factor, but while this can cover the problem of the amount of intercepted rainfall and surface runoff, adjusting for the site is not readily possible with this approach. Furthermore, we are forced to distribute daily rainfall events as hourly input over the whole day, thereby manipulating the timing of the rainfall onset. For example, on day 279 there is still some sap flux and evaporation measured even though a rainfall event happened probably later in the day. As the modeled storage immediately after rainfall events overestimates the water content, it can be concluded that the model somewhat oversimplifies the water infiltration due to rainfall due to these limitations.

A third reason could be the missing stem water potential measurements. From the 2009 period it became clear that when giving about equal weight to each measurement type in the objective function, the agreement between all three modeled and measured series increased. The stem water potential holds valuable information to estimate the hydraulic parameters of the tree, thus not including them might provide insufficient information to find the best parameters.
5.3. Vertical Water Fluxes

The transport of water is governed by vertical flow processes, both in the soil and the tree. Figure 9 shows vertical fluxes averaged over segments of certain length and, for the tree, time periods. In the soil, fluxes are mostly downwards in 2009 with some upwards movement near the surface, and strongly downwards in 2010 due to dominating rainfall pattern. In both years, a peak of less downwards flow can be seen around -100 cm depth. This is the maximum of the root density distribution (see Figure 4), leading locally to water being transported into this region to replace water taken up by roots.

In the tree, water is transported upwards into the canopy. Above 600 cm, water is extracted from sink terms along the tree nodes, and the vertical flux reaches a peak, that gradually goes down towards zero. The vertical fluxes in 2010 exhibit similar behavior as the 2009 ones, but with smaller absolute values, due to the smaller potential evapotranspiration. Vertical flux is clearly higher during the hours between 8 am and 4 pm, and the decrease after the peak is stronger.

(...)?more depending on converged results???

6. Summary and Outlook

TEXT

7. Appendix

??Find out how to restart figure numbering after appendix environment so this doesn’t have do be a section.??
This section describes the literature data used for the comparison of the tree hydraulic functions in Figs. 10 to 14. Waring and Running (1978) analysed the sapwood of tall Douglas Firs from the Cascade Mountains of Oregon. They measured relative water content in the laboratory, and related them to water potential measurement and the relative change in conductivity that was estimated from measurements of transpiration. This data set was presented as relative conductivity against saturation, so we translate this data set into vulnerability curves using our best parameter sets.

From the thesis of Yoder (1984), we included measurements on a White Fir. Twig samples were taken from young trees (10-13 years old) and a water retention curve was measured in the laboratory using a pressure bomb technique as established by (Tyree and Hammel, 1972). Measurements were taken at different times over year, and we include data from March, June and August.

A number of branches of mature tree specimen were analysed using hydraulic conductivity and acoustic measurements by Cochard (1992b) to investigate vulnerability to air embolism and cavitation. From his data, we include vulnerability curve measurements on a Douglas Fir.

Sperry and Ikeda (1997) compared air-injection and dehydration methods for determining the vulnerability curves of conifers. As both methods were found to obtain similar results, we restrict the data included to White Fir dehydration measurements on branch segments (10-20 cm long).

A comparison of the vulnerability curves for outer and inner sapwood on young (1.0-1.5 m tall) and mature Douglas firs (41-45 m tall) was included.
(Domec and Gartner, 2001), as well as a vulnerability curves established through a centrifugal method as described by Li et al. (2008).

To allow some comparison to other tree species, we also include newer results by Gonzalez-Benecke et al. (2010) and Johnson et al. (2011) that establish vulnerability curves on Red Maple, American Tulip Trees, Virginia Pines, Slash Pines and Longleaf Pines.

References


ation of a low-cost soil water content sensor for wireless network applications. Journal of Hydrology 344, 32–42.


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Figure 1: Site scheme. The six pits with soil moisture probes used for this study are marked with blue circles.

Figure 2: Schematics of the model.
Figure 3: Scheme of water flow boundary processes.

Figure 4: Optimized root density distribution (2009 period) to a depth of 2.5 m.
Figure 5: Water stress response function $\alpha(h)$ and characteristic pressure values.

Figure 6: Initial pressure head distribution in the soil for the 2009 period.
Figure 7: Example of a slice of the objective function for two parameters and the evolution of two chains. Only 12 positions are shown for each chain, evenly spaced in time. The thicker arrows marks the first jump.
Figure 8: Caterpillar plot
Figure 9: Vertical fluxes averaged over segments of 50 cm (soil) or 300 cm (tree) length. (c) and (d) in the lower row are segmented in time for hours between 8 am and 4 pm or other hours. The segmented data was approximated by a smoothing spline.
Figure 10: Vulnerability curves 2009. Median of optimized posterior distribution as thick green line, blue area gives 95% confidence interval. Literature data: (×) White Fir (Waring and Running, 1978), (▲) Inner Sapwood, 1 m (▼) Inner Sapwood, 35 m (♦) Outerwood Sap, 1 m (■) Outer Sapwood, 35 m - Douglas Fir (Domec and Gartner, 2001), (×) White Fir, Dehydration (Sperry and Ikeda, 1997), (+) Red Maple, (▲) American tulip tree, (▼) Virginia Pine (Johnson et al., 2011), (♦) Slash Pine, (■) Longleaf Pine (Gonzalez-Benecke et al., 2010), (+) Douglas Fir (Cochard, 1992b), (×) White Fir (Li et al., 2008).
Figure 11: Vulnerability curves 2010. Median of optimized posterior distribution as thick green line, blue area gives 95% confidence interval. Literature data: (×) White Fir (Waring and Running, 1978), (▲) Inner Sapwood, 1 m (▼) Inner Sapwood, 35 m (♦) Outerwood Sap, 1 m (■) Outer Sapwood, 35 m - Douglas Fir (Domec and Gartner, 2001), (×) White Fir, Dehydration (Sperry and Ikeda, 1997), (+) Red Maple, (▲) American tulip tree, (▼) Virginia Pine (Johnson et al., 2011), (♦) Slash Pine, (■) Longleaf Pine (Gonzalez-Benecke et al., 2010), (+) Douglas Fir (Cochard, 1992b), (×) White Fir (Li et al., 2008).
Figure 12: Extract of the distance correlation matrix for the 2009 parameter posterior distributions. Larger and more intensely red circle represent a large correlation.
Figure 13: Soil Water Characteristics 2009. Median of optimized posterior distribution as thick green line, blue area gives 95% confidence interval. Literature data: (■) White Fir (Waring and Running, 1978), (+) White Fir, March (▲) June (▼) August (Yoder, 1984).
Figure 14: Soil Water Characteristics 2010. Median of optimized posterior distribution as thick green line, blue area gives 95% confidence interval. Literature data: (■) White Fir (Waring and Running, 1978), (+) White Fir, March (▲) June (▼) August (Yoder, 1984).
Figure 15: Forcing, modeled and measured data for 2009 optimization.
Figure 16: Forcing, modeled and measured data for 2010 optimization.
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Table 2: Prior parameter range and posterior parameter 50 % and 95 % confidence interval for 2010 period.

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