SSDA Code to Apply Data Assimilation in Soil Water Flow Modeling:

Documentation and User Manual

Gonzalo Martinez[1,2], Feng Pan[2], and Yakov Pachepsky[1]

[1]Environmental Microbial and Food Safety Laboratory
Beltsville Agricultural Research Center
USDA-ARS
[2]University of Cordoba, Spain
[3]Energy and GeoScience Institute, University of Utah

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Abstract

Soil water flow models are based on simplified assumptions about the mechanisms, processes, and parameters of water retention and flow. That causes errors in soil water flow model predictions. Data assimilation (DA) with the ensemble Kalman filter (EnKF) corrects modeling results based on measured state variables, information on uncertainty in measurement results and uncertainty in modeling results. The purpose of this manual is to describe the application of DA with EnKF into soil water flow modeling to improve simulation results. The DA with EnKF code was developed to assimilate the data of soil water content measurements at one or more depths with the ensemble of models (e.g., pedotransfer functions (PTFs) for water retention function and saturated hydraulic conductivity (Ksat) in soil water flow modeling). The DA with EnKF code written in FORTRAN was coupled with HYDRUS-1D code as soil water flow modeling tools. The manual describes the DA with EnKF theory, the soil water flow model, and contains detailed instructions for input and output data, and sample problems.

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1. Introduction

A large number of soil water flow and storage models have been developed for applications in hydrology, meteorology, agronomy, contaminant hydrology, and other fields. Each of these models is based on a set of simplified assumptions about the mechanisms, processes, and parameters of water retention and flow, and it is often not possible to predict whether a particular set of assumptions will be applicable for a specific site. Therefore, errors in soil water modeling predictions arise that result from both conceptual uncertainty and the lack of detailed knowledge about model parameters.

Using monitoring data to periodically correct modeling results is a way to reduce modeling errors. The correction consists in updating simulated values, i.e. replacing simulated values of environmental variables with values that are closer to the measured ones. This operation is called data assimilation (DA). It has become a common approach in modeling atmospheric and oceanic systems (Lahoz et al., 2010)

The simplest way of data assimilation is the direct insertion of the measured values of state variables in place of simulated ones. Although this DA method has been applied from time to time (Houser et al., 1998; Walker et al., 2001a,b; Heatman et al., 2003), it has been recognized that DA-based correction of modeling results should use information on uncertainty in data and uncertainty in modeling results. Simulated values should be changed to the values very close to measured ones if the uncertainty in data is much less than the uncertainty in modeling results. On the other hand, there is no reason to substantially change simulated values if the uncertainty in modeling results is much less than the uncertainty in data. This concept has been formalized by applying the statistical technique called Kalman filter which is a proven data assimilation method for linear dynamics and measurement processes with Gaussian error statistics (Kalman, 1960). This technique has been applied from the very beginning of data assimilation in soil moisture modeling (Aboitiz et al., 1986; Or and Hanks, 1992). As the data assimilation for nonlinear models became of interest, the ensemble Kalman filter (EnKF) was proposed by Evensen (1994) to overcome limitations of Kalman filter. The EnKF is a sequential data assimilation method, which uses an ensemble of model states to represent the error statistics of the model estimation. The idea is to start an ensemble of (many) simulations by varying model parameters, initial state variables, and forcing within feasible ranges. The variation in modeling results within the ensemble at the time of state variable update is used to define the uncertainty in modeling results.

Vereecken et al. (2008) noted that the conceptual simplicity, relative ease of implementation, and computational efficiency of the EnKF make the method an attractive option for data assimilation in vadose zone hydrology. The EnKF has been proven to be an efficient approach to correct Richards equation-based soil flow modeling results of soil water contents by assimilating surface soil moisture (Das and Mohanty, 2006).

Selection of the ensemble of models can strongly affect the efficiency of data assimilation with EnKF. It was recently proposed to build an ensemble of soil water flow simulations using an ensemble of pedotransfer functions, or PTFs (Guber et al., 2005, 2008, 2009). The argument went that the accuracy of PTF outside the data collection region is essentially unknown, and the ensemble forecasts offer a way of filtering the predictable from the unpredictable through averaging – the features that are consistent among ensemble members are preserved, while those that are inconsistent are reduced in amplitude. Perhaps more important, the ensemble itself, as a sample from possible forecast outcomes, can be used to estimate the forecast uncertainty and the likely structure of forecast errors (Hamill et al., 2003). Pedotransfer functions were used to adjust the spatial distribution of soil texture and hydraulic properties to match simulated and measured soil moisture when the direct insertion of remotely sensed surface soil water content was used as the data assimilation method (Santanello et al., 2007). However, pedotransfer functions have not been so far used in soil water sensor data assimilation.

The purpose of this manual is to describe the application of coupled DA and EnKF with PTFs as ensemble into soil water flow modeling to improve simulation results. The DA with EnKF code was developed to assimilate the data of soil water content measurements at one or more depths with the ensemble of models (e.g., pedotransfer functions (PTFs) for water retention function and saturated hydraulic conductivity (Ksat) in soil water flow modeling). The DA with EnKF code written in FORTRAN was coupled with HYDRUS-1D code as soil water flow modeling tools. This manual describes the DA with EnKF theory, the soil water flow model, detailed instructions for input and output data, and sample problems.

2. Theory

2.1. Ensemble Kalman Filter

The Kalman Filter is an implementation of the Bayesian update method. Given a probability density function (pdf) of the state of the modeled system (the prior) and the

probability distribution function of data, the Bayes theorem is used to obtain the PDF after the data has been taken into account (the posterior). The Bayesian update incorporates new data when they become available, and model advances in time from one update to another. The following description is based on the work of Mandell (2007).

The Kalman filter relies on the normal distributions of data and modeling results. Let the model for any simulated time generate N state variables $x_1, x_2, \ldots x_{n.,}$ The probability distribution function $p(x)$ of the vector of simulation results $\mathbf{x}=\{ x_1, x_2, \ldots x_{n.}\}$ is

$$p(\mathbf{x}) = A_1 \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \mathbf{Q}^{-1}(\mathbf{x}-\boldsymbol{\mu}) \right) \qquad (1)$$

where $\boldsymbol{\mu}$ is the vector of mean values of variables x_1, x_2,, x_n, $\mathbf{Q}$ is the covariance matrix, A_1 as well as A_2, A_3, and A_4 in equations below, are scaling multipliers to have the integral of probability distribution function equal to one. The function $p(\mathbf{x})$ is the prior probability distribution on the moment the state has to be updated to account for data. The vector of data values $\mathbf{d}$ is also assumed to be normally distributed with the mean $\bar{\mathbf{d}}$ and covariance matrix $\mathbf{R}$. It is assumed that the mean data vector $\bar{\mathbf{d}}$ is related to state variables $\mathbf{x}$ via matrix $\mathbf{H}$ as $\bar{\mathbf{d}} = \mathbf{Hx}$. The value $\mathbf{Hx}$ is what the value of the data would be for the state $\mathbf{x}$ in the absence of data errors. Then the probability density $p(\mathbf{d}|\mathbf{x})$ of the data $\mathbf{d}$ conditional of the system state $\mathbf{x}$, is

$$p(\mathbf{d}\,|\,\mathbf{x}) = A_2 \exp\left(-\frac{1}{2}(\mathbf{d}-\mathbf{Hx})^T \mathbf{R}^{-1}(\mathbf{d}-\mathbf{Hx}) \right) \qquad (2)$$

For the update purposes, one needs the probability density of states conditioned on data $p(\mathbf{x}\,|\,\mathbf{d})$ rather than the probability density of data conditioned on states $p(\mathbf{d}\,|\,\mathbf{x})$. The conversion of $p(\mathbf{d}\,|\,\mathbf{x})$ to $p(\mathbf{x}\,|\,d)$ can be done using the Bayes theorem

$$p(\mathbf{x}\,|\,\mathbf{d}) = A_3\, p(\mathbf{d}\,|\,\mathbf{x})\, p(\mathbf{x}) \qquad (3)$$

States conditioned on data, i.e. $\mathbf{x}|\mathbf{d}$, are posterior states, they are referred below as x^p. When (1) and (2) are used to compute the right-hand side of (3), the expression for $p(\mathbf{x}^p)$ is obtained in the form:

$$p(\mathbf{x}^p) = A_3 \exp\left(-\frac{1}{2}(\mathbf{x}^p - \boldsymbol{\mu}^p)^T \mathbf{Q}^{p\,-1}(\mathbf{x}^p - \boldsymbol{\mu}^p) \right) \qquad (4)$$

The posterior mean $\boldsymbol{\mu}^p$ and posterior covariance Q^p in Eq. (4) are given by the Kalman update formulas:

$$\boldsymbol{\mu}^{\mathbf{p}} = \boldsymbol{\mu} + \mathbf{K}(\mathbf{d} - \mathbf{H}\boldsymbol{\mu})$$
$$\mathbf{Q}^{\mathbf{p}} = (\mathbf{I} - \mathbf{KH})\mathbf{Q} \qquad (5)$$

where

$$\mathbf{K} = \mathbf{QH}^{\mathbf{T}}(\mathbf{HQH}^{\mathbf{T}} + \mathbf{R})^{-1} \qquad (6)$$

is the Kalman update matrix. The Kalman update changes state variables taking into account (a) data available at the moment when predictions have been obtained, (b) the accuracy of those data, and (c) variability of state variables. One important feature of the Kalman filter is that the number of elements (measurements) in the data vector **d** is usually much smaller than the number of state variables – elements of the vector **x**.

The ensemble Kalman filter (EnKF) has been developed to overcome the difficulty of using the original Kalman filter in cases when the dependence of the covariance matrix **Q** on time is difficult to find. The EnKF estimates the covariance matrix as the sample covariance computed from the ensemble simulation results. The ensemble is composed from randomly generated equiprobable realizations of the studied model. The randomness may apply to initial conditions, model parameters, and boundary conditions or forcing.

Let the ensemble consists of *N* models and each model predicts *n* state variables. Let the predictions of the i^{th} model form the vector $\boldsymbol{x}_i$ that has *n* elements $\boldsymbol{x}_{i,}$ *i=1,2,…n,* which are predicted values of state variables. The *n* x *N* matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_N]$ is the prior ensemble. The goal is to correct the predictions at each of preset update times by changing this matrix to the posterior ensemble $\mathbf{X}^p = [\mathbf{x}_1^p, \mathbf{x}_2^p, ...\mathbf{x}_N^p]$. It is assumed that the data form the vector **d** that has *m* elements. The vector **ε** is the random error in data characterized by the *m* x *m* error covariance matrix **R.**

The ensemble Kalman filter (or EnKF) update consists of four basic steps.

1. Find the *n* x *N* covariance matrix **C** of ensemble predictions $\mathbf{x}_i$
2. Generate representative random data separately for each ensemble member: $\mathbf{d}_1=\mathbf{d}+\boldsymbol{\varepsilon}_1$, $\mathbf{d}_2=\mathbf{d}+\boldsymbol{\varepsilon}_2$, …, $\mathbf{d}_N=\mathbf{d}+\boldsymbol{\varepsilon}_N$, where the random vector **ε** belongs to the *n*-dimensional normal distribution *N*(0,R).
3. Collect the random data in the *m* x *N* matrix $\mathbf{D}=[\mathbf{d}_1,\mathbf{d}_2,\ldots\mathbf{d}_N]$
4. Find the corrected predictions as:

$$\mathbf{X}^{\mathrm{p}}=\mathbf{X}+\mathbf{K}(\mathbf{D}-\mathbf{Hx}) \qquad (7)$$

where the Kalman gain matrix K relates the variability in predictions and the data accuracy and is estimated as

$$\mathbf{K= CH^T(HCH^T+R)^{-1}} \quad (8)$$

The one-dimensional case gives a general feel of how the ensemble Kalman filter works. Consider the case n=1 and m=1 when there is only one model-predicted state variable and its value is measured. All matrices then will become scalars, and **H** will be equal to 1. Let $x_i=\mu+\xi_i$, ξi belongs to $N(0,\ \sigma_x^2)$, and $d_i=d+\varepsilon_i$, ε_i belongs to $N(0, \sigma_d^2)$. The gain K will be

$$\mathrm{K} = \frac{\sigma_x^2}{\sigma_x^2 + \sigma_d^2} \quad (9)$$

and

$$x_i^p = (1 - \mathrm{K})(\mu + \xi_i) + \mathrm{K}(d + \varepsilon_i) \quad (10)$$

Values of K are between 0 and 1. The value of x_i^p is close to x_i when K is close to zero, i.e. $\sigma_d^2 >> \sigma_x^2$ and accuracy in data is much lower compared with the variability in predictions. On the contrary, the value of x_i^p is close to d_i when K is close to one, i.e. $\sigma_x^2 >> \sigma_d^2$ and accuracy in data is much higher than the variability in predictions.

2.2. Soil Water Flow Model

The one-dimensional vertical soil water flow was simulated with the Richards equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial \mathrm{z}}\left[K(\theta)\left(\frac{\partial h}{\partial \mathrm{z}} + 1\right)\right] \quad (11)$$

where: θ is the soil water content [$L^3\ L^{-3}$]; h is the matric potential [L]; K is the hydraulic conductivity [$L\ T^{-1}$]; z is the vertical axis directed upward [L]; t is the time [T]. Soil water retention was described using the van Genuchten equation (van Genuchten, 1980):

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left[1 + (\alpha \mid h \mid)^n\right]^m} \quad (12)$$

where: θ_s, θ_r are saturated and residual soil water content [$L^3\ L^{-3}$]; α [L^{-1}], n, m are van Genuchten water retention parameters. The hydraulic conductivity was computed from the van Genuchten-Mualem equation (van Genuchten, 1980):

$$K = K_{sat}\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^l\left\{1-\left[1-\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{1/m}\right]^m\right\}^2 \quad (13)$$

where: K_{sat} is saturated hydraulic conductivity [L T^{-1}], l is an empirical shape-defining parameter. The value of the parameter m was set to 1-1/n.

Equation 11 was solved numerically using the HYDRUS 1D numerical procedures (Šimůnek et al., 2008).

2.3. Pedotransfer Functions to Develop the Ensemble of Models

Pedotransfer functions developed from large databases were used to generate parameters in the van Genuchten-Mualem parameterization of soil hydraulic properties in variably saturated soils (Eqs.12 and 13). Parameters of the water retention function (Eq.12) could be found from any functions (e.g., Table 1 of Guber and Pachepsky, 2010). Several sets of K_{sat} values could be used to create ensembles of models (e.g., statistical values of K_{sat}; Rawls et al., 1998; Schaap and Leij, 1998; Carsel and Parrish, 1998; Wösten et al., 1999 etc.). The ensemble of many models (number of water retention PTFs × number of K_{sat} PTFs) is applied in soil moisture data assimilation with EnKF.

2.4. Temporal Stability of Water Contents and Data Bias Estimates

The random error in data has to be characterized to apply the Kalman update method. Because the time series at the same depths were correlated, the 'naive' computation of the covariance matrix of data errors D under the assumption of independence of data in different locations at the same depth could result in large inaccuracies (Wigley et al., 1984) since correlated observations result in inflated type 1 errors (Quinn and Keough, 2002). Therefore, the statistical model of the data was assumed in the form (Jacques et al., 2001):

$$\theta_{i,j}(t) = \mu_i(t) + b_{i,j} + \eta_{i,j} \quad (14)$$

where i is the subscript to denote depth, i=15, 35, 55, 75, 95 cm, j is the subscript to denote location across the trench, j=1,2,…,12, μ_i is the average water content at the depth "i", $b_{i,j}$ is the bias of the measurement in location j at the depth "i" relative to the average water content at this depth, and η_{ij} is the random component that is used to define the covariance matrix.

2.5. Interpolation of Assimilation Results in Soil Profile

One specific feature of the assimilation algorithm in this work is that assimilation is performed for the small number of depths rather than for each depth of the finite element grid covering the soil profile. Results of data assimilation are then interpolated across the soil profile assuming linear dependences of logarithms of pressure heads on depths between interpolation points. The top and the bottom pressure heads obtained from simulations are preserved to perform the linear interpolation outside of the range of measurement depths at all assimilation times. The assimilation depths set includes the measurement depths set.

The initial water contents for simulations are set at assimilation depths. The initial distribution of water contents across profile is constructed by linear interpolation between the initial water content depths and linear extrapolation outside of the range of initial water content depths.

3. Data Assimilation Code

3.1. Source Files and Executable

The version 6.0 of the HYDRUS1D code (Simulnek et al., 1998), called HYDRUS6 below, has been used in this work.

The source code files are listed in the Table 3.1 below.

Table 3.1. Source files of the SSSA code.

File name	Description
DA_SSDA.for	Data assimilation routine based on the Ensemble Kalman filter
INPUT.FOR	HYDRUS6 data input routines
MATERIAL.FOR	HYDRUS6 data input routines
OUTPUT.FOR	HYDRUS6 output routines
SINK.FOR	HYDRUS6 sink term computation routine
SOLUTE.FOR	HYDRUS6 solute transport routine
SSDA.FOR	Main program including HYDRUS6 converted to the subroutine.
TEMPER.FOR	HYDRUS6 heat transport routine
TIME.FOR	HYDRUS6 simulation time step control routines
WATFLOW.FOR	HYDRUS6 water flow routine
w_to_h.for	Initial water content interpolation routine
w_to_h_b.for	Water content interpolation after data the assimilation update

The executable files are ‘SSDA64.exe’ and ‘SSDA32.exe’ for 64 bit and 32 bit Windows systems, respectively.

The ‘datadir.txt’ file has to be in the same directory as an executable. It contains the path to the directory where input and output files are to be found.

3.2. Input Files

Input file ‘Input.dat’ includes names of the following input files:

- observation data for each of measurement depths
- temporal stability-based sensor bias values for each location and depth
- initial water contents at all data assimilation depths
- initial water contents at all data assimilation depths
- template to build the HYDRUS6 input file ‘Profile.dat’

- template to build the HYDRUS6 input file ‘Atmosph.in’
- template to build the HYDRUS6 input file ‘Selector.in’

Content of each of above files is detailed below in Tables 3.2-3.8. All input files are in ASCII format. Note that descriptions of the three templates are available in HYDRUS 1D manuals and included in this manual for the convenience.

The data assimilation code SSDA uses HYDRUS6 to simulate 1D water flow in soil profile. The proper work of SSDA was tested only for atmospheric top boundary conditions and either free drainage or constant head bottom boundary conditions in absence of root activity. HYDRUS6 is capable to simulate much wider variety of boundary conditions and sink terms, as well as solute and heat transport. We have not tested these capabilities in data assimilation projects, although this is undoubtedly possible. SSDA uses unmodified input files of HYDRUS6 where input of variables referring to all capabilities of HYDRUS6 is preserved. Dummy variables are used in SSDA to provide inputs that HYDRUS6 requires but does not use in SSDA applications.

Table 3.2 ‘Input.dat’ file content

Item #	Line #	Variable	Description
1	1	Title	Title and comments
2	2	Comment line	
3	3	*ntobs*	Total number of measurement times in observed water content time-series
4	3	*ndepth*	Total number of assimilation depths
5	3	*nsensor*	Total number of water content sensors at measurement depths
6	3	*nmat*	Total number of materials in the profile
7	4	Comment line	
8	5	*Depths(i)* (*i*=1,*ndepth*)	Depths where data assimilation occurs
9	6	Comment line	
10	7	*ipick*(i), *i*=1,*ndepth*	Data availability indicator: if larger than zero, then measurements are available at the depth ‘*i*‘
11	8	Comment line	
12	From 9 to 8+*NMD*	Filenames of measurements for each depth where measurements are available	File names for water content time series data, total of *NMD* files where *NMD* is the number of measurement depths, i.e. the total number of positive values in the *ipick* array.

Table 3.2. (Continued)

Item #	Line #	Variable	Description
13	9+*NMD*	Comment line	
14	10+*NMD*	Filename	Name of the temporal stability bias file
15	11+*NMD*	Comment line	
16	12+*NMD*	Filename	Template to build the HYDRUS6 input file 'Profile.dat'
17	13+*NMD*	Filename	Template to build the HYDRUS6 input file 'Atmosph.in'
18	14+*NMD*	Filename	Template to build the HYDRUS6 input file 'Selector.in'
19	15+*NMD*	Comment line	
20	16+*NMD*	*NDAtimes*	Total number of DA update time intervals
21	17+*NMD*	Comment line	
22	18+*NMD*	*DAtimes*(*i*), *i=1,NDAtimes*+1	DA update times
23	19+*NMD*	Comment line	
24	20+*NMD*	*NPTF*	Total number of PTFs = the total numbre of models in the ensemble
25	21+*NMD*	Comment line	
26[¶]	22+*NMD*	*PTFid*	The ID number of PTF function as listed in Table 1 of the CalcPTF code manual (Guber and Pachepsky, 2010, this website)
27	22+*NMD*	*imodtype*	0, van Genuchten-Mualem parameters, 2 – Brooks-Corey parameters
28	22+*NMD* to 22+*NMD*+*nmat*	*thr*	Residual water content for each of soil materials
29	22+*NMD* to 22+*NMD*+*nmat*	*ths*	Saturated water content for each of soil materials
30	22+*NMD* to 22+*NMD*+*nmat*	*alpha*	Parameter α in case of van Genuchten-Mualem model (if *imodtype* = 0), air entry pressure in case of Brooks-Corey model (if *imodtype* = 2)
32	22+*NMD* to 22+*NMD*+*nmat*	*vgn*	Parameter *n* in case of van Genuchten-Mualem model (if *imodtype* = 0), parameter λ in case of Brooks-Corey model (if *imodtype* =2)
33	22+*NMD* to 22+*NMD* +*nmat*	*aks*	Saturated hydraulic conductivity
34	22+*NMD* to 22+*NMD* +*nmat*	*al*	Tortuosity parameter

[¶]Items 26 through 34 are repeated to provide information for each of *NPTF* pedotransfer function

Table 3.3. Observation data for each of measurement depths

Line #†	Variable	Description
1 to *ntobs*	*tobs*	Day of the year to the beginning of which soil water content data are available
1 to *ntobs*	*Wnew* (*i*), *i*=1,*nsensors*)	Soil water contents for all sensors at this measurement

Table 3.4. Temporal stability-based sensor bias values for each location and measurement depth

Line #†	Variable	Description
1 to *NMD*	Bias	Bias values for all sensors at depths where measurements are available

Table 3.5. Initial water contents at data assimilation depths

Line #	Variable	Description
1 to *ndepth*	*winit1*	Soil water content corresponding to the first observation time in the Table 3.3

Table 3.6. Template to build the HYDRUS6 input file 'Profile.dat'

Line #	Variable	Description
1	*n*	Number of fixed nodes, set equal to 2 in SSDA
2		Top fixed node, use values from the test example
3		Bottom fixed node, use values from the test example
4	*NumNP*, *nnodes*	Total number of nodes
4	NS	Number of solutes, set to 0
From 5 to 4+*nnodes*	n	Node number
From 5 to 4+*nnodes*	*x*(*n*)	*x*-coordinate of the node
From 5 to 4+*nnodes*	*hNew*	Initial value of the pressure head at node *n.* An arbitrary number in SSDA
From 5 to 4+*nnodes*	*MatNum*	Soil material at node *n*
From 5 to 4+*nnodes*	*LayNum*	Subregion number at node *n*, set equal to *MatNum* in SSDA
From 5 to 4+*nnodes*	*Beta*	Value of the water uptake distribution, set equal to zero in SSDA
From 5 to 4+*nnodes*	*Ax*	Nodal value of the pressure head scaling factor, set equal to 1 in SSDA
From 5 to 4+*nnodes*	*Bx*	Nodal value of the hydraulic conductivity scaling factor, set equal to 1 in SSDA
From 5 to 4+*nnodes*	*Dx*	Nodal value of the watder content scaling factor, set equal to 1 in SSDA

Table 3.7. Template to build the HYDRUS6 input file 'Atmosph.in'.

Line #	Variable	Description
1	Comment line	
2	Comment line	
3	*MaxAL*	Total number of days when precipitation, evaporation and transpiration data are available.
4	Comment line	
5	*hCritS*	Maximum allowed pressure head on soil surface
6	Comment line	
From 7 to 6+*MaxAL*	*tAtm*	Day of the year, is used as the first day in simulations
From 7 to 6+*MaxAL*	*Prec*	Daily precipitation
From 7 to 6+*MaxAL*	*rSoil*	Daily surface evaporation
From 7 to 6+*MaxAL*	*rR*	Potential daily transpiration
From 7 to 6+*MaxAL*	*hCA*	Absolute value of the minimum pressure head on soil surface
From 7 to 6+*MaxAL*	*rB*	Daily bottom flux (set equal to zero if *KodBot* is positive, or if one of logical variables *qGWLF*, *FreeD* or *SeepF* is **"true"**, see settings in the 'Selector_template.in' file),
From 7 to 6+*MaxAL*	*hB*	Groundwater level, or any other prescribed pressure head boundary condition as indicated by a positive value of *KodBot* (set equal to 0 if *KodBot* is negative, or if one of the logical variables *qGWLF*, *FreeD* or *SeepF* is **"true".**, see settings in the 'Selector_template.in' file)
From 7 to 6+*MaxAL*	*hT*	Prescribed pressure head at the surface (set equal to 0 if *KodBot* is negative, see settings in the 'Selector_template.in' file)
From 7 to 6+*MaxAL*	*tTop*	Temperature on the surface[¶]
From 7 to 6+*MaxAL*	*tBot*	Temperature at the bottom of the soil profile[¶]
From 7 to 6+*MaxAL*	*Ampl*	Amplitude of temperature fluctuations [¶]
From 7 to 6+*MaxAL*	*cT*	Concentration at the surface [¶]
From 7 to 6+*MaxAL*	*cB*	Concentration at the bottom[¶]

Table 3.8. Template to build the HYDRUS6 input file 'Selector.in'.

Line #	Variable	Description
1	Comment line	
2	Comment line	
3	*Hed*	Heading
4	Comment line	
5	*LUnit*	Length unit (e.g., 'cm').
6	*TUnit*	Time unit (e.g., 'min').
7	*MUnit*	Mass unit for concentration (e.g., 'g', 'mol', '-').

[¶]Set equal to zero in SSDA applications

Table 3. 7. (Continued)

Line #	Variable	Description
8	Comment line	
9	*lWat*	Set this logical variable equal to **.true.** when transient water flow is considered. Set this logical variable equal to **.false.** when initial condition is to be kept constant during the simulation.
9	*lChem*	Set this logical variable equal to **.true.** if solute transport is to be considered.
9	*lTemp*	Set this logical variable equal to **.true.** if heat transport is to be considered.
9	*lSink*	Set this logical variable equal to **.true.** if water extraction from the root zone occurs.
9	*lRoot*	Set this logical variable equal to **.true.** if root growth is to be considered.
9	*lShort*	**.true.** if information is to be printed only at preselected times, but not at each time step, **.false.** if information is to be printed at each time step.
9	*lWDep*	**.true.** if hydraulic properties are to be considered as temperature dependent, false. otherwise
9	*lScreen*	**.true.** if information is to be printed on the screen during code execution.
9	*AtmInf*	**.true.** if variable boundary conditions are supplied via the input file ATMOSPH.IN, **.false.** if the file ATMOSPH.IN is not provided (i.e., in case of time independent boundary conditions).
9	*lEquil*	**.true.** if equilibrium or no adsorption is considered in the solute transport equation, **.false.** if nonequilibrium adsorption is considered for at least one solute species.
9	*lInverse*	**.true.** if inverse problem is to be solved, **.false.** if direct problem is to be solved.
10	-	Comment line.
11	*NMat, MatNum*	Number of soil materials
11	*Nlay*	Number of subregions
11	*CosAlpha*	Cosine of the angle between the vertical line and the water flow
12	Comment line	Comment line
13	Comment line	
14	*MaxIt*	Maximum number of iterations allowed during any time step (usually 20).

Table 3.7. (continued)

Line #	Variable	Description
14	*TolTh*	Absolute water content tolerance for nodes in the unsaturated part of the flow region (its recommended value is 0.0001). *TolTh* represents the maximum desired absolute change in the value of the water content between two successive iterations during a particular time step.
14	*TolH*	Absolute pressure head tolerance for nodes in the saturated part of the flow region (its recommended value is 0.1 cm). *TolH* represents the maximum desired absolute change in the value of the pressure head between two successive iterations during a particular time step.
15	Comment line	
16	*TopInf*	**.true.** if time dependent boundary condition is to be imposed at the top of the profile; data are supplied via input file ATMOSPH.IN, **.false.** in the case of time independent surface boundary conditions.
16	*WLayer*	Set equal to **.true.** if water can accumulate at the surface with zero surface runoff.
16	*KodTop*	Code specifying type of boundary condition (BC) for water flow at the surface. Code number is positive for Dirichlet BC and negative for Neumann BC. In the case of 'Atmospheric BC' set *KodTop*=-1. Set KodTop=0 when a prescribed BC can change from Dirichlet BC to Neumann BC and vice versa.
16	*lInitW*	Set equal to **.true.** if the initial condition is given in terms of the water content. Set equal to **.false.** if the initial condition is given in terms of the pressure head
17	Comment line	
18	*BotInf*	**.true.** if time dependent boundary condition is to be imposed at the bottom of the profile; control data are supplied via input file ATMOSPH.IN, **.false.** in the case of time independent bottom boundary conditions.
18	*qGWLF*	Set equal to **.true.** if the discharge-groundwater level relationship is applied as bottom boundary condition.
18	*FreeD*	**.true.** if free drainage is to be considered as bottom boundary condition.
18	*SeepF*	**.true.** if seepage face is to be considered as the bottom boundary condition.
18	*KodBot*	Code specifying type of boundary condition for water flow at the bottom of the profile. Code number is positive for a Dirichlet BC and negative for a Neumann BC. In case of a seepage face or free drainage BC set *KodBot*=-1.

Table 3.7. (Continued)

Line #	Variable	Description
18	*DrainF*	**.true.** if flow to horizontal drains is considered as bottom boundary condition.
19	Comment line	
20	*hTab1*	Absolute value of the upper limit of the pressure head interval below which a table of hydraulic properties will be generated internally for each material (*hTab1* must be greater than 0.0; e.g. 0.001 cm)
20	*hTabN*	Absolute value of the lower limit of the pressure head interval above which a table of hydraulic properties will be generated internally for each material (hTabN must be fairly large, e.g. 100000 cm)
21	Comment line	
22	*iModel*	Soil hydraulic properties model ID. This entry is not used in SSDA application, it s read a *imodtype* from the Input.dat file
22	*iHyst*	Hysteresis in the soil hydraulic properties. Set to zero in the current SSDA applications, = 0; No hysteresis
23	Comment line	
From 24 to 23+nMat	Par(1,M)	Residual water content for soil material M=Line number -23
From 24 to 23+nMat	Par(2,M)	Saturated water content for soil material M=Line number -23
From 24 to 23+nMat	Par(3,M)	Parameter α in case of van Genuchten-Mualem model (if *imodtype* = 0) , air entry pressure in case of Brooks-Corey model (if *imodtype* = 2); for soil material M=Line number -23
From 24 to 23+nMat	Par(4,M)	Parameter *n* in case of van Genuchten-Mualem model (if *imodtype* = 0) , parameter λ in case of Brooks-Corey model (if *imodtype* =2); for soil material M=Line number -23
From 24 to 23+nMat	Par(5,M)	Saturated hydraulic conductivity for soil material M=Line number -23
From 24 to 23+nMat	Par(6,M)	Tortuosity parameter for soil material M=Line number -23
24+NMat	Comment line	
25+NMat	Comment line	
26+NMat	*dt*	Initial time increment, *dt*. Initial time step should be estimated in dependence on the problem being solved. For problems with high-pressure gradients (e.g. infiltration into an initially dry soil), *dt* should be relatively small
26+NMat	*dtMin*	Minimum permitted time increment
26+NMat	*dtMax*	Maximum permitted time increment

Table 3.7. (continued)

Line #	Variable	Description
26+NMat	*dMul*	If the number of required iterations at a particular time step is less than or equal to *ItMin*, then *dt* for the next time step is multiplied by a dimensionless number *dMul* ≥ 1.0 (its value is recommended not to exceed 1.3).
26+NMat	*dMul2*	If the number of required iterations at a particular time step is greater than or equal to *ItMax*, then dt for the next time step is multiplied by *dMul2* ≤ 1.0 (e.g. 0.33).
26+NMat	*ItMin*	If the number of required iterations at a particular time step is less than or equal to ItMin, then dt for the next time step is multiplied by a dimensionless number *dMul* ≥ 1.0 (its value is recommended not to exceed 1.3).
26+NMat	*ItMax*	If the number of required iterations at a particular time step is greater than or equal to *ItMax*, then *dt* for the next time step is multiplied by *dMul2* ≤ 1.0 (e.g. 0.33).
26+NMat	*MPL*	Number of specified print-times at which detailed information about the pressure head, water content, flux, temperature, concentrations, and the water and solute balances will be printed
28+NMat	*tInit*	Initial time of the simulation, make sure it is the same or larger than the first time in the Atmosph.in file if atmospheric boundary conditions are imposed
28+NMat	*tMax*	Final time of the simulation, make sure it is the same or smaller than the last time in the Atmosph.in file if atmospheric boundary conditions are imposed
29+NMat	-	Comment line.
29+NMat	TPrint(i), i=1,MPL	HYDRUS6 print times

3.3 Output Files

SSDA creates two groups of output files – data assimilation output files and HYDRUS6 output files. The data assimilation files are described below. Descriptions of HYDRUS6 output files A_LEVEL.OUT, BALANCE.OUT, I_CHECK.OUT, NOD_INF.OUT, OBS_NODE.OUT PROFILE.OUT, RUN_INF.OUT, and T_LEVEL.OUT. can be found in the HYDRUS6 manual (Simunek e al., 1998).

Simulation results for each data assimilation depth for each time step are printed to files sim_**.txt where ** stands for the number of PTF used in the order set in the Input.dat file. Measured water contents are provided for the beginning of each day in files wout_obs***.txt where *** stands for depth in cm. Simulated water contents are provided for the beginning of

each day in files wout_sum***.txt where *** stands for depth in cm. Note that measured water contents are given for measurement depths, and simulated water contents are given data assimilation depths.

4. Sample Problem

The sample problem was selected to apply the DA code to research how effective assimilation of soil water content sensor data can be in correcting simulated soil water content profiles in field soils. The ensemble of models was developed with six pedotransfer functions (PTFs) for water retention and four PTFs for the saturated hydraulic conductivity (K_{sat}). The included example refers to data assimilation from three depths.

4.1 Soil Water Content Monitoring Data

The experimental setup and soil water content data have been previously described by Jacques (2000) and Pachepsky et al. (2005). In brief, the experimental field was located at Bekkevoort, Belgium. It was situated at the bottom of a gentle slope and was covered with a meadow. The soil was classified as Eutric Regosol (FAO, 1975). A trench, 1.2 m deep and 8 m long, was dug at the field site. The grass cover was removed from the experimental area. A plastic sheet to isolate the disturbed trench zone covered one side of the trench. Volumetric water content was measured with time domain reflectometry (TDR). Sixty two-rod TDR probes (25 cm long, 0.5 cm rod diameter, 2.5 cm rod spacing) were installed along the 5.5 m of the trench at 12 locations each 50 cm at 5 depths of 15, 35, 55, 75, and 95 cm (Fig. 1). Soil texture and organic matter content were measured in samples taken where the probes were installed. Grain-size analyses of the sand samples have been performed according to the European standard EN 933-1. Soil texture was sandy loam at depths of 15 cm, 35 cm, and 55 cm, and loam at depths of 75 cm and 95 cm. One measurement cycle for all TDR-probes took approximately 35 minutes, and the time difference between two measurements for the same probe was 2 hours. After all devices were installed, the trench was filled. Rainfall was continuously measured at the site with a rainfall recorder (200 cm^2) with a floated pen system on a paper (0.1 mm interval, rotation speed 1 cm h^{-1}). Other meteorological parameters were obtained from the station 3 km from the site. A thin layer of gravel (1 to 2 cm) was evenly distributed on the study area. Field measurements

started on March 11, 1998 (day 0) and finished on March 31, 1999 (day 384). The site-specific TDR calibration (Jacques, 2000) was used.

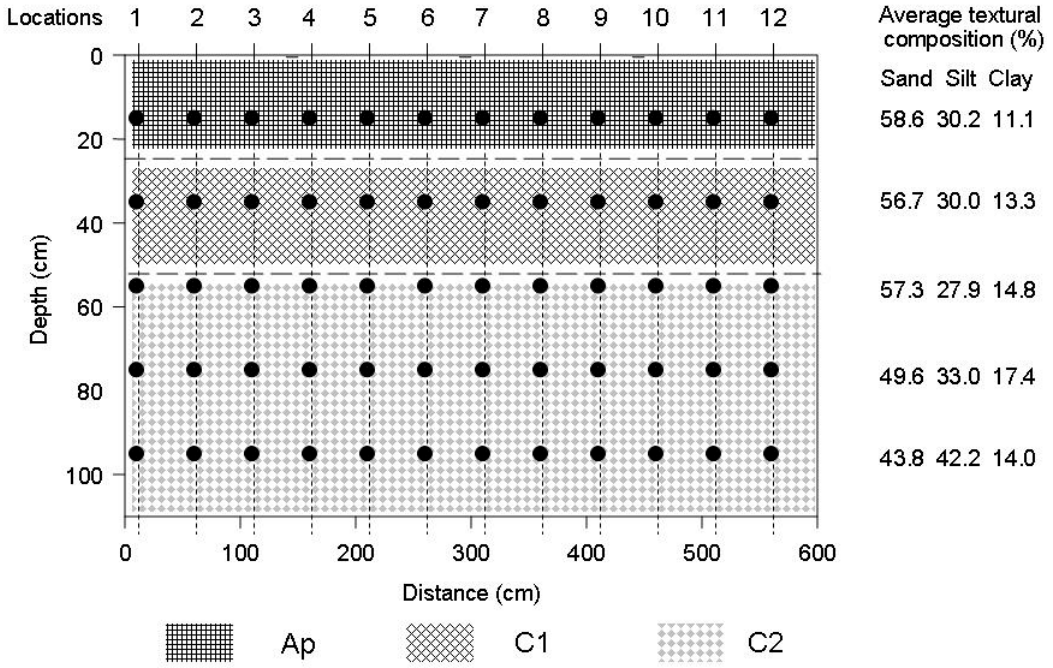

Fig. 1. Time domain reflectometry probe placement (•) at the trench wall. Locations one through 12 denote twelve positions along the trench where sets of 5 sensors – one for each measurement depths were installed. Filled rectangles show Ap, C1, and C2 horizons top to bottom. Dashed lines show the average position of the horizon boundary, and white bands show the observed range of horizon boundary depths. Average values of clay, silt, and sand content are given for the probe installation depths. Adopted from (Pachepsky et al. 2005)

4.2 Soil Water Flow Model Setup

Hydrus-1D software was used to simulate the soil water flow in the site. The atmospheric boundary with daily rainfall and evapotranspiration was set as the top boundary condition, and the free drainage boundary condition was set as the bottom boundary condition. The pressure head profile calculated from measured soil water content based on the van Genuchten equation was set as the initial condition. Predicted and updated state variables were water contents at five measurement depths averaged across the 12 observation locations at the beginning of the day of update.

4.3 Ensemble of Models Built with Pedotransfer Functions

Pedotransfer functions developed from large databases were used to generate parameters in the van Genuchten-Mualem parameterization of soil hydraulic properties in variably saturated soils (Eqs.12 and 13). Parameters of the water retention function (Eq.12) were found from the six pedotransfer functions (Table 4.1) developed from the European continental data base HYPRES (Wösten et al., 1999), subsets of the US nationwide database (Gupta and Larson, 1979; Rawls et al., 1983), the nationwide Brazilian dataset (Tomasella and Hodnett, 1998), and the large national Hungarian database in which sandy loam and loam soils were well represented (Rajkai and Varallyay, 1992). The pedotransfer equations of water retention parameters are described in details in Guber and Pachepsky (2010).

Four sets of K_{sat} values were used to create ensembles of models in this sample problem (Table 4.2). The K_{sat} values were estimated (a) based on textural class and bulk density according to the table developed from a large US nationwide database (Rawls et al., 1998), (b) as the average values of K_{sat} found from three large databases (Schaap and Leij, 1998), (c) from clay and sand contents with regression equations developed from a large dataset of Soil Conservation Service (SCS) Soil Survey Information Reports (Carsel and Parrish, 1988), and (d) from fitting the van Genuchten-Mualem equation to geometric mean water contents developed using the European continental database HYPRES (Wösten et al., 1999). The ensemble of 24 models (6 PTFs of water retention × 4 K_{sat} PTFs) was applied in soil moisture data assimilation with EnKF.

Table 4.1. Soil water retention PTFs with estimated van Genuchten parameters.

Parameter	PTFs	Wösten et al. (1999)	Wösten et al. (1999)	Tomasella and Hodnett (1998)	Gupta and Larson (1979)	Rajkai and Varallyay (1992)	Rawls et al. (1983)
		VG[¶]	VG[¶]	WH→VG[§]	WH→VG[§]	WH→VG[§]	WH→VG[§]
Model							
Clay (%)		+			+	+	+
Silt (%)		+	+	+	+		+
Sand (%)		+	+	+	+	+	+
OC (%)			+	+	+	+	+
BD (gcm^{-3})			+		+	+	+
VG α (1/m)	15cm	0.0249	0.0436	0.1705	0.0281	0.0084	0.0532
	35cm	0.0314	0.0404	0.1118	0.0405	0.0064	0.0477
	55cm	0.0314	0.0450	0.1034	0.0488	0.0061	0.0527
	75cm	0.0314	0.0394	0.0734	0.0353	0.0059	0.0394
	95cm	0.0314	0.0280	0.0515	0.0192	0.0062	0.0300
VG *n*	15cm	1.1689	1.2214	1.2097	1.4158	1.1827	1.2916
	35cm	1.1804	1.2537	1.2173	1.3566	1.1672	1.3455
	55cm	1.1804	1.2593	1.2339	1.3385	1.1820	1.3567
	75cm	1.1804	1.2376	1.2318	1.3188	1.1214	1.3474
	95cm	1.1804	1.2548	1.2259	1.3680	1.0737	1.3539

[¶]Parameters of the van Genuchten equation are estimated with the pedotransfer function
[§]Water contents at specific pressure heads are estimated, and then the van Genuchten equation is fitted to the estimates.

Table 4.2. Saturated hydraulic conductivity from literature PTFs.

No.	Reference	Saturated Hydraulic Conductivity ($cm\ d^{-1}$)	
		Sandy Loam	Loam
1	Rawls, et al. (1998)	55.0	12.5
2	Schaap and Leij (1998)	38.0	12.0
3	Carsel and Parrish (1988)	106.0	25.0
4	Wösten et al. (1999)	12.1	10.8

4.4 Data Assimilation Results

The developed DA code was used to simulate the soil water content profile between Day 100 (April 10, 1998) and Day 247 (September 4, 1998). Selected data assimilation results are shown in Fig. 2. Data assimilation provided an excellent update of weekly simulation results when the data from all depths were assimilated (Fig. 2a). Inspection of graphs in Figs. 2b and 2c shows that assimilation of measurements from the depth of 15 cm resulted in the same accuracy as assimilation of data from all depths and assimilation of measurements from the depth of 95 cm resulted in relatively large errors in the top of the profile. While the update was satisfactory, the simulations between update times deviated from measurements since parameters of the model were not changed.

Results of daily data assimilation are shown in Fig. 3. The daily update prevents the development of the simulation bias that has been well pronounced with weekly updates (Fig. 2). Using the data from only one depth corrects results throughout the profile in case of daily updates as in a case of less frequent updates. However, utilizing more than one sensor seems to be beneficial, since the use of only one sensor from the 15-cm depth leads to the exaggeration of water content dynamics at larger depths (Fig. 3b), and the use of the sensor from the 90-cm depth does not properly correct the simulated dynamics at 15 cm and 35 cm depths. The RMSE values for daily assimilation are substantially – up to 12 times - less than in the case of weekly simulations. The best overall result has been achieved when all 5 sensors have been used. The next best overall results have been obtained with pairs of sensors from 15 cm and 55 cm, and from 35 cm and 95 cm.

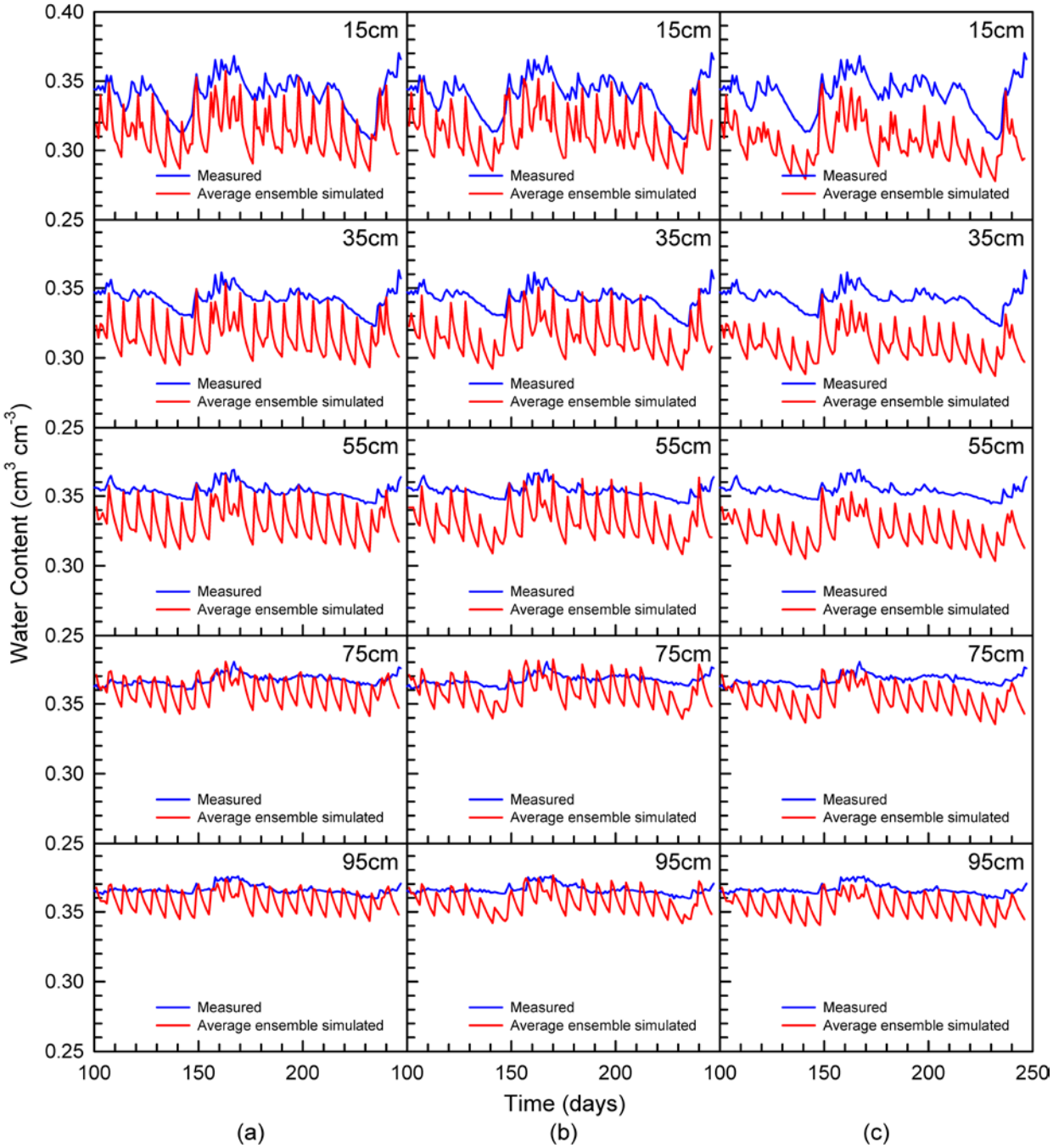

Fig. 2. Selected results of weekly ensemble simulations update; (a) update with assimilation of data from sensors from all five depths, (b) update with assimilation of data from sensors at the 15-cm depth, and (c) update with assimilation of data from the sensors at the 95-cm depth.

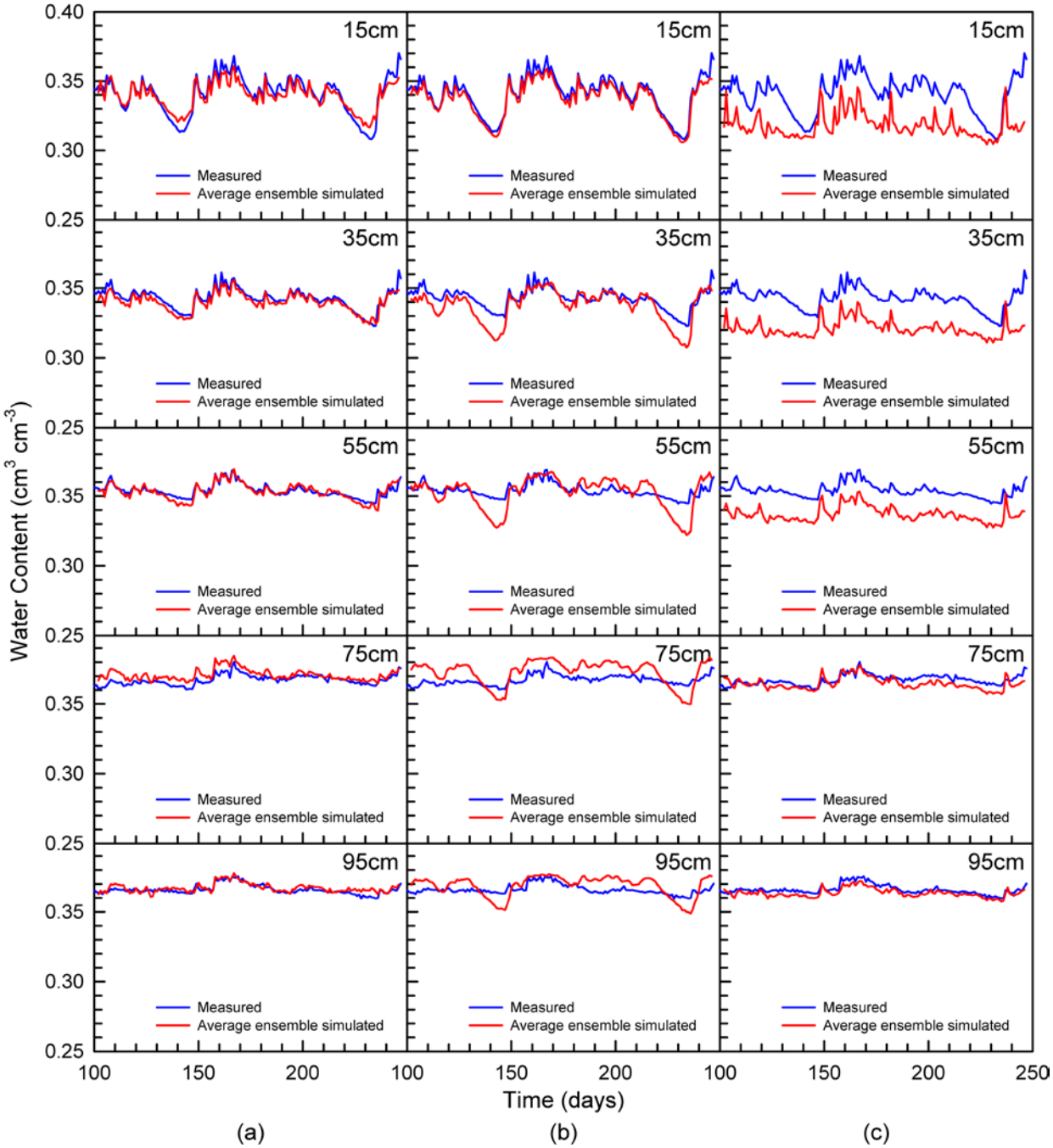

Fig. 3. Selected results of daily ensemble simulations update; (a) update with assimilation of data from sensors from all five depths, (b) update with assimilation of data from sensors at the 15-cm depth, and (c) update with assimilation of data from the sensors at the 95-cm depth.

5. Conclusions

This manual outlines the code that combines the ensemble Kalman filter-based data assimilation with the developments in pedotransfer functions, temporal stability of soil water patterns, and soil water content sensors. The code was developed to facilitate improvements in modeling results in soil hydrology and related fields. The sample problems demonstrates that assimilation of soil water content sensor data appears to be effective in correcting soil water content profiles simulated with the Richards equation based model; small number of sensors was sufficient to correct the simulated profile. The developed code can also be applied into the modeling accuracy improvement in various hydrology-related fields.

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