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Characterization, controlling, and reduction of uncertainties in the modeling and observation of land-surface systems

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Uncertainty is one of the greatest challenges in the quantitative understanding of land-surface systems. This paper discusses the sources of uncertainty in land-surface systems and the possible means to reduce and control this uncertainty. From the perspective of model simulation, the primary source of uncertainty is the high heterogeneity of parameters, state variables, and near-surface atmospheric states. From the perspective of observation, we first utilize the concept of representativeness error to unify the errors caused by scale representativeness. The representativeness error also originates mainly from spatial heterogeneity. With the aim of controlling and reducing uncertainties, here we demonstrate the significance of integrating modeling and observations as they are complementary and propose to treat complex land-surface systems with a stochastic perspective. In addition, through the description of two modern methods of data assimilation, we delineate how data assimilation characterizes and controls uncertainties by maximally integrating modeling and observational information, thereby enhancing the predictability and observability of the system. We suggest that the next-generation modeling should depict the statistical distribution of dynamic systems and that the observations should capture spatial heterogeneity and quantify the representativeness error of observations.

uncertainty, data assimilation, scale, observability, predictability, model, remote sensing

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Land-surface systems are giant, open, complex systems (Qian, 1991) that, accordingly, require a clear mathematical framework with respect to achieving quantitative meta-syntheses in the study of such a system.

The modeling and observation of Earth systems are two fundamental methods that are employed to understand these systems, and these two areas have witnessed rapid development in the past two decades; in particular, Earth observation systems have advanced our understanding of the systems on Earth into a new era. However, for land-surface systems, much uncertainty remains with regard to correctly reconstructing the history of change and predicting shortterm and long-term changes. It is clear that this uncertainty is one of the greatest challenges in the quantitative understanding of land-surface systems.

Fundamental questions include the following: where does this uncertainty originate? Is it inherent, or can we not eliminate such uncertainty due to an insufficient understanding? Since such uncertainty exists, can the land-surface process be accurately simulated and predicted? All these questions are related to our understanding of the inherent characteristics of land-surface systems. As Einstein stated, "God does not throw dice"; Bohr replied, "Einstein, do not tell God what to do"¹⁾. Indeed, the debate in classical phys-

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¹⁾ In a 1926 letter to Max Born, Einstein wrote: "I, at any rate, am convinced that He [God] does not throw dice."

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ics over the past century reminds us of the following: Shall we treat the complicated geographical world (e.g., the land-surface system) around us based on the ideal of certainty or from a stochastic perspective? If the geographic world around us is random and is intrinsically uncertain, what type of methods should we use to address and control this uncertainty to enhance the observability and predictability of land-surface systems?

By analyzing the uncertainty in the modeling and observation of land-surface systems, this paper attempts to rationalize the methodology that plays a key role in the modern scientific study of Earth systems, namely the data assimilation or model assimilation of data. We will also attempt to demonstrate how the data assimilation method treats and controls uncertainty by maximizing the integration of modeling and observational information and thereby enhances the predictability and observability of the system.

1 Sources of uncertainty

1.1 The temporal and spatial heterogeneity of model elements: a water cycle example

Let us first analyze the uncertainty caused by the temporal and spatial heterogeneity of model elements through a typical example in terrestrial hydrology.

The movement of water in unsaturated soil is generally expressed by Richards' equation (Richards, 1931), and its one-dimensional expression in the vertical direction of the soil profile is written as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right],\tag{1}$$

where θ (m³ m⁻³) is the water content, ψ (m) is the water potential, *K* (m s⁻¹) is the hydraulic conductivity, *z* (m, upward as positive) is the soil depth, and *t* (s) is time.

Richards' equation achieves very good results in the prediction of soil moisture at microscopic scales and has been well validated by numerous observational facts at microscopic scales. Therefore, a large number of land-surface models and hydrological models adopt this equation as the governing equation for soil water movement. However, there is always a large error in the simulation results of soil moisture with macroscopic applications from the basic model unit (usually a grid) to a catchment and then to the global scale. Is this because the governing equation is incorrect or because there are other reasons?

First, we should discuss whether Richards' equation satisfies the scale invariance. In the past two decades, despite controversy with regard to this question, it is mostly agreed that Richards' equation has a mathematical form at the macroscopic scale that is consistent with the microscopic scale, though the hydraulic conductivity needs to be redefined as an effective or equivalent parameter (Kabat et al., 1997; Yang et al., 2000). When we apply Richards' equation to a model grid of a land surface model or a hydrological model, by default, it is scale invariant. Therefore, we assume that:

(1) Richards' equation (structure of the model) is correct and is applicable to various scales.

(2) The hydraulic conditions are non-homogeneous in the grid.

(3) The possible error caused by numerical computation is negligible because it is not related to the inherent uncertainty of dynamic processes.

Thus, from the perspective of spatial heterogeneity, temporal variation, and observability on both microscopic and macroscopic scales, the model parameters, model state variables, and boundary conditions were sequentially analyzed to identify the sources of model uncertainty.

(i) Parameters

The parameter in eq. (1) is the hydraulic conductivity K, which has a strong spatial heterogeneity and can vary by more than three orders of magnitude within a short distance (Jarvis et al., 2002). Because K is a function of the soil moisture content, it also changes over time with the soil moisture content; particularly during the process of freeze-thaw cycle, K can vary more than several orders of magnitude within a short time. K is observable at the microscopic scale. However, due to the presence of preferential flow (such as micropore flow), the macroscopic hydraulic conductivity is not equal to the average of multiple microscopic observations and instead is always larger than it. Therefore, K is almost unobservable at model grid scale or at other macroscopic scales. Strictly speaking, the microscopic measurement of the hydraulic conductivity only provides us with a reference to estimate a macroscopic quantity, whereas estimating the representative value on a grid or at another macroscopic scale requires reference to other information. Therefore, we can conclude that K has a strong spatial and temporal heterogeneity and the heterogeneity is the primary source of uncertainty when Richards' equation is applied at the macroscopic scale.

(ii) State variables

In eq. (1), the soil water content θ is the state variable in Richards' equation, and the sources of uncertainty can also be analyzed from the aforementioned four aspects. Although θ might vary significantly within a very small range, the intensity of its spatial variation is weaker than *K*; thus, θ can be considered to have moderate spatial heterogeneity. θ also shows significant variations over time and can be observed on microscopic scales; however, it remains difficult to observe soil moisture on a grid and at other macroscopic scales. Therefore, it is difficult to provide correct initial fields for soil moisture in the model.

(iii) Boundary conditions (forcing)

Without a loss of generality, Richards' equation can be discretized as a specific model for multi-layered water flow. For example, the governing equations of water balance in the revised Simple Biosphere model (SiB2) (Sellers et al., 1996) are as follows:

$$\frac{\partial \theta_1}{\partial t} = \frac{1}{D_1} \left[P - Q_{1,2} - \frac{1}{\rho_w} E_g \right], \tag{2}$$

$$\frac{\partial \theta_2}{\partial t} = \frac{1}{D_2} \left[Q_{1,2} - Q_{2,3} - \frac{1}{\rho_w} E_{tr} \right], \tag{3}$$

$$\frac{\partial \theta_3}{\partial t} = \frac{1}{D_3} [Q_{2,3} - Q_3], \tag{4}$$

where θ_i (*i*=1, 2, 3) (m³ m⁻³) is the volumetric water content of each soil layer, D_i (m) is the soil thickness of each layer, P (m s⁻¹) is the precipitation rate, $Q_{1,2}$ and $Q_{2,3}$ (m s⁻¹) are the water fluxes between the *i*th and the (*i*+1)th layers in the soil, Q_3 (m s⁻¹) is the gravitational drainage, E_g and E_{tr} (m s⁻¹) are the evaporation flux and canopy transpiration flux, respectively, and ρ_w (kg m⁻³) is the water density. Other land surface models and hydrological models adopt a similar method to describe the process of soil water flow.

The third source of uncertainty, namely the uncertainty of atmospheric forcing in a land-surface model, which determines the boundary conditions of Richards' equation, is further discussed below. In the above equations, the upper boundary condition is related to precipitation, evaporation, runoff, and snowmelt, and the lower boundary condition is related to the gravitational drainage (Zeng and Decker, 2009). The boundary conditions, e.g., evaporation, are also related to the state of the near-surface atmosphere, including wind, temperature, pressure, humidity, and radiation. The various states of near-surface atmosphere that determine the upper boundary condition of Richards' equation are collectively referred to as atmospheric forcing, which usually has a weak to moderate spatial heterogeneity, though the temporal variation is strong. In general, the representative space of atmospheric forcing is larger than those of parameters and state variables and thus is considered to be observable at macroscopic scales. However, the uncertainty related to the spatial representativeness of atmospheric forcing will inevitably be transferred to the simulation results when Richards' equation is employed.

According to the analysis of the examples above, even if the model itself is perfect and the physical structure of the model does not rely on the scale, that is, the same laws of physics can be applied to both microscopic and macroscopic scales, the uncertainty of model parameters, initial conditions of the model state, and boundary conditions will still be reflected in the simulation results of models through complicated error propagation. The uncertainty of these three elements is also closely related to their strong spatial and temporal heterogeneity, particularly the spatial heterogeneity.

Therefore, the following corollaries regarding the uncer-

tainty of models can be made:

(1) The kinetic mechanism at microscopic scale of many land surface processes is known, whereas the parameters, state variables, and boundary conditions that affect these processes have high heterogeneity in space and time. In this situation, upscaling a dynamic process at the microscopic scale to the macroscopic scale (such as a grid or a catchment) will result in significant uncertainty. This uncertainty is not caused by an unknown process but rather originates from the spatial and temporal heterogeneity of the parameters, state variables, and boundary conditions and the associated scale effect.

(2) The model uncertainty is inherent and typically can be estimated, controlled, and reduced. However, because heterogeneity always exists, it cannot be eliminated completely.

(3) The accurate estimation of parameters, state variables, and boundary conditions at macroscopic scales can only be defined on a statistical basis. If a parameter or variable is a 'true value', it is defined as the unbiased estimate, namely, the mathematical expectation of its representativeness error at the macroscopic scale is zero, and its uncertainty (defined by the second order statistical moment, such as variance) can be controlled within an expected range. This is our mathematical definition of model uncertainty.

In addition, we can deduce the following corollaries.

The parameters in the land surface model must be calibrated. These parameters are usually not observable at macroscopic scales, though well-designed observation has great significance. Such observations can provide the probability distribution of the parameters and the constraint conditions on the upper and lower boundaries of the parameters. These distribution characteristics and constraint conditions are important a priori information for parameter estimation.

1.2 Representativeness error of in situ observations

The error of *in situ* observations can be decomposed into instrument and representativeness errors. In general, after the instrument is stringently calibrated, the systematic error of the measurement will be eliminated and the measurement error tends to be a random error so that its uncertainty can be quantitatively characterized with such statistical quantities as variance.

Therefore, we presume that the instrument has been calibrated in the discussion of the uncertainty of *in situ* observations. Additionally, based on the definition of 'true value' in the previous section, we assume that

(1) The measurement error of a certain instrument is a random error and its uncertainty (e.g., in terms of variance) is known.

(2) As the mathematical expectation of random error is 0, we can presume that the instrument measurement is the 'true value' of the object to be measured at the observation time and within its representative space.

The representativeness error is then analyzed as follows. The representative space of in situ observations has the following features: (1) It varies for the different variables or parameters to be observed (hereafter referred to as 'param $eter')^{2}$. For example, the representative space of the time-domain reflectometer (TDR) that measures soil moisture is generally on the scale of a centimeter to tens of centimeters, the representative space of a solar radiation observation instrument is approximately ten times its erection height (on the order of decameter), and the representative space of an eddy covariance system is generally on the scale of hundreds of meters. (2) It varies for different methods of observation; for example, for the observations of soil moisture, there is a significant difference among the representative spaces of sampling and drying, TDR measurement, and the method of cosmic ray measurement. (3) It varies with time, and the representative space of observations is a function of itself and the variables and parameters that impact it; as all these parameters change with time, the representative space of observations is also a function of time.

As observed, due to the heterogeneity of the land surface, the representative space of any type of observation is not matched to the simulation unit of the model (such as grid, hydrological response unit, and catchment). This means that it is a complicated question to extrapolate observational results to a specific model unit or, conversely, to convert the state variable on the model unit to the observed value in a specific representative space with a given error estimate.

We define the relationship that maps the model state on a specific model unit to the observed values in the representative space of an observation as the observation operator, and the measurement of its uncertainty as the representativeness error. Obviously, the representativeness error is closely related to the spatial heterogeneity, and it needs to be defined on a statistical basis. Therefore, if the spatial heterogeneity cannot be effectively captured and its statistical characteristics (probability density distribution function in space and time) be correctly characterized, the spatial unit transformation between the model state and *in situ* observations will not be effectively achieved.

Accordingly, the following corollaries regarding the uncertainty of *in situ* observations can be made:

(1) The *in situ* observation can only (when the instrument error is very small and the instrument has been calibrated) obtain the 'true value' of the object to be measured at the observation time and within its represented space, and there is a significant representativeness error when the observation is transformed to another spatial unit.

(2) The representativeness error of *in situ* observations is closely related to the spatial heterogeneity.

(3) The characterization of representativeness error should capture the features of the spatial and temporal vari-

ations of the object to be measured at a macro-scale, and these features are the main basis for the estimation of representativeness error.

1.3 Representativeness error of remote sensing observations

Remote sensing has achieved great success and yet is still fraught with many uncertainties (NRC, 2008). Retrieving land surface parameters from remote sensing involves two methods: inversion and model estimation. An example of the former includes retrieving the leaf area index from canopy reflectance, and an example of the latter is to use parameters retrieved from remote sensing, such as land surface temperature, albedo, soil moisture, and leaf area index, as the model input to estimate evapotranspiration.

Both methods rely on raw remote sensing observations, such as albedo and radiative temperature. Compared to inversed quantities and estimators, the raw observation is generally more reliable and only subject to relatively small instrument error, without systematic error after rigorous calibration. In addition, the raw remote sensing observation obtains an ensemble of information regarding radiation in its representative space (pixel or footprint), and it intrinsically contains the heterogeneity of the radiation characteristics in its representative space. Therefore, it can be defined that the raw remote sensing observation does not have representativeness error.

However, to understand the various processes in landsurface systems, the raw remote sensing observations need to be transformed to parameters of land surface; furthermore, it is necessary to transform the observations to the spatial unit matched to the dynamic model. The representativeness error caused by the latter transformation is similar to the representativeness error of *in situ* observations, as discussed in the section 1.2. Here, the focus is on the representativeness error caused by the former transformation.

The model that maps land-surface parameters to the raw remote sensing observations is typically referred to as the forward radiative transfer model (i.e., observation operator), and its inverse model is termed as the inversion model. The error of inversion models is very complicated and involves whether the model is invertible and the effective use of *a priori* information. To simplify the discussion, the uncertainty of remote sensing is explored only from the perspective of forward models, and the error of the forward radiative transfer model is defined as the representativeness error of remote sensing observations.

Ideally, the forward radiative transfer model should be a macroscopic model. However, although there is an ongoing attempt to develop macroscopic models at the pixel scale (Li et al., 1999), most models only consider the heterogene-

²⁾ There is a clear distinction between the definition of variable and parameter in the dynamic model; in contrast, there is no need to deliberately distinguish between variable and parameter for observation systems; for the purpose of convenience, the term 'parameter' is used collectively herein.

ity in the vertical direction, with some of them considering the heterogeneity at relatively microscopic scales, such as the modeling of surface roughness in the microwave radiative transfer model. As for heterogeneity at macroscopic scales, most radiative transfer models generally assume scale invariance for the physical structure. In summary, the following approaches are utilized in the radiative transfer modeling at the pixel scale:

(1) A homogeneous pixel is assumed, meaning that the structure and parameters of the forward model are scale invariant.

(2) The model structure is scale invariant but effective or equivalent parameters are used as the input for the forward model.

(3) Monte Carlo simulation or real scene modeling is used. We define this method as the parameter ensemble approach; namely, an ensemble of parameters is used to replace the statistical population.

(4) The macroscopic model is developed or redeveloped (Li et al., 1999, 2000).

Because surface heterogeneity always exists, obviously, it is not possible for the first approach to build a real microscopic model. For all other approaches, strictly speaking, the characteristics of the spatial distribution of parameters need to be known at the pixel scale. However, at the pixel scale, because of the nonlinear characteristics of the parameters, nonlinear characteristics of the radiative transfer model, and the interaction of parameters, the heterogeneity of various parameters in the pixel obviously cannot be linearly superposed. Therefore, to both obtain the equivalent parameter and establish the radiative transfer model at the macroscopic scale, one of the main factors to be considered is the spatial heterogeneity of the parameters. In summary, although the ways of macroscopic modeling are different, the error caused by the scale representativeness of parameters in the forward radiative transfer model can be attributed to representativeness error. By defining the representativeness error as above, we unify the uncertainty of in situ observations and remote sensing observations with respect to the concept of error.

Therefore, by making the following presumptions:

(1) The instrument error of remote sensing sensors is a random error, and its quantity (such as variance) is known.

(2) The mathematical error of radiative transfer models to be solved can be ignored and is not related to the inherent uncertainty caused by the heterogeneity on the pixel scale.

The following corollaries regarding the uncertainty of remote sensing observations can be made:

(1) Original remote sensing observations have inherent heterogeneity and do not have representativeness error.

(2) The representativeness error of the remote sensing forward model is mainly from the spatial heterogeneity of the parameters within the pixel scale.

(3) Even the forward model takes into account heterogeneity; however, from the perspective of inversion, it will cause the number of parameters to be inverted far more than that of the observations, forming an ill-posed inversion. Therefore, it is necessary to develop new inversion strategies and introduce new information; otherwise the model will not be able to derive the equivalent value of the parameters at the pixel scale from the raw observations with intrinsic heterogeneity.

2 How to reduce and control uncertainty

2.1 Complementation of model and observations

Both the models and observations of land-surface systems have significant uncertainty, though it is unclear whether the superposition of uncertainty will lead to greater uncertainty. Furthermore, if the answer is negative, it is unclear how the uncertainty can be reduced and controlled.

In section 1, the respective uncertainty of the model and observations was analyzed, demonstrating complementarity: the model provides a unified dynamic framework for the continuous evolution of land-surface systems in time and space, though it contains uncertainty caused by the intrinsic heterogeneity; the observation, after a strict calibration, provides the true value for the observation time and the representative space. However, there is a relatively significant representativeness error for the transformation of an observation into other spatial units and the mapping between the model state and observations.

Can we possibly use the complementary relationship between models and observations to reduce and control this uncertainty? The development of cybernetics has actually provided a sophisticated mathematical tool for this purpose. As commented by Xuesen Qian, "...cybernetics is a theory of relationship" (Qian, 1957), thus the relationship between models and observations needs to be studied.

The integration of observation and model simulation can be analyzed as an analogy to a classic application of a cybernetic missile. The reason that the missile can accurately hit its target is that, in addition to its own dynamic features (analogous to a model), more importantly, it continuously captures information that is fed back to the trajectory of the missile and constantly adjusts the trajectory based on the observational information. Thus, the missile will eventually accurately hit its target only if the observations are correct. What should be noted is that it is vital to evaluate the uncertainty of the observations, which is the problem of error estimation. It can be imagined that, if the system cannot make an effective judge on the false information, it will cause the missile to deviate completely from its target.

The relationship between dynamic models and observations is analogous to the aforementioned example, and the fusion between them is called data assimilation, which is considered to be a strategy for the Earth system sciences (NRC, 1999). The data assimilation method differs from the traditionally standalone model simulation by the following: in the data assimilation, the model will constantly monitor the relevant observational information and establish the relationship between the model state and direct or indirect observations (i.e., the observation operators mentioned in sections 1.2 and 1.3); the observation information, after quality control, is then integrated into the model trajectory via a feedback mechanism and is used as the basis for adjusting the model trajectory. The essence of data assimilation is: The true value of observation at the observation time and within its representative space is used to calibrate the model, and the model expands this information to a time and space that are more continuous and complete.

A definition for data assimilation can be given as follows (Talagrand, 1997; Li et al., 2007): data assimilation is the method that, within the framework of dynamic models, integrates direct and indirect observations at different scales and from different sources and continuously optimizes the model trajectory based on weighted errors of both dynamic models and various observations to reduce the error of the whole system.

2.2 Data assimilation algorithm

What type of mathematical methods does data assimilation use to fuse observation and model information? In general, the modern data assimilation adopts two types of methods: the optimization method and the sequence filtering derived from modern cybernetics.

The optimization method is employed to link the model, observations, and their respective errors through an objective function. It applies various types of optimization methods to minimize this objective function to obtain an optimized model trajectory.

With the state space representation, Richards' equation in section 1.1 or other dynamic models can be generalized as a nonlinear model, M, which is called the model operator. X_0 represents the initial conditions of the model state and is a column vector comprised of various state variables, with the subscript 0 meaning the initial state. X_0^b is the background field, which is the a priori knowledge of the model state; B is the covariance matrix of the model error. The observation operator is expressed as H_i , where the subscript *i* is time, meaning H may change with time; R_i is defined as the covariance matrix of observation error, which is the sum of instrument error and representativeness error. The observation at time *i* is expressed as Y_i^o , which could be the same physical quantities as X (direct observation) or other quantities with different physical meaning from X (indirect observation).

From the least-squared estimate, maximum likelihood estimate, or based on Bayes' Theorem, we can deduce that the optimal fusion of the model and observations is expressed as follows:

$$J(\boldsymbol{X}_{0}) = \frac{1}{2} (\boldsymbol{X}_{0} - \boldsymbol{X}_{0}^{b})^{T} B^{-1} (\boldsymbol{X}_{0} - \boldsymbol{X}_{0}^{b}) + \frac{1}{2} \sum_{i=0}^{n} (H_{i} \{ [\boldsymbol{M}(\boldsymbol{X}_{0})]_{i} \} - \boldsymbol{Y}_{i}^{o})^{T} R_{i}^{-1} (H_{i} \{ [\boldsymbol{M}(\boldsymbol{X}_{0})]_{i} \} - \boldsymbol{Y}_{i}^{o}),$$
(5)

where *J* is the objective function. The optimized model trajectory can be obtained by minimizing the function above. *J* is the integration of three types of information, including the dynamic model *M*, observation information (*H* and Y°), and the errors of the model and observations (*B* and *R*).

Another type of data assimilation methods is the filtering method, which includes various Kalman filtering and particle filtering methods. Bayesian filtering, as a more general form of these methods (Li and Bai, 2010), integrates the information of model and observations based on considering the errors through two procedures of prediction and update, and thus reduces the uncertainty of the entire system.

Here, the forecast procedure is expressed as

$$p(\boldsymbol{X}(t_{k}) | \boldsymbol{Y}^{o}(t_{1:k-1})) = \int p[\boldsymbol{X}(t_{k}) - \boldsymbol{M}_{k}(\boldsymbol{X}(t_{k-1}))] p(\boldsymbol{X}(t_{k-1}) | \boldsymbol{Y}^{o}(t_{1:k-1})) d\boldsymbol{X}(t_{k-1}),$$
(6)

The update procedure is expressed as

$$p(\boldsymbol{X}(t_{k}) | \boldsymbol{Y}^{o}(t_{1:k})) = \frac{p[\boldsymbol{Y}^{o}(t_{k}) - H_{k}(\boldsymbol{X}(t_{k}))]p(\boldsymbol{X}(t_{k}) | \boldsymbol{Y}^{o}(t_{1:k-1}))}{\int p[\boldsymbol{Y}^{o}(t_{k}) - H_{k}(\boldsymbol{X}(t_{k}))]p(\boldsymbol{X}(t_{k}) | \boldsymbol{Y}^{o}(t_{1:k-1}))d\boldsymbol{X}(t_{k})}, \quad (7)$$

where p is the probability density function and t_k or the subscript k means the time k. The meaning of the other symbols is the same as in eq. (5).

Bayesian filtering integrates three types of information: (1) information on the dynamic evolution of systems, i.e., the model operator M_k ; (2) observational information, which includes all the observations before time k, $\mathbf{Y}^{o}(t_{k})$, and the observation operator H_k ; and (3) error information, which includes the model error $p[X(t_k) - M_k(X(t_{k-1}))]$ and the observational error $p[Y^{\circ}(t_k) - H_k(X(t_k))]$. As an estimate of uncertainty, the error plays a significant role in the fusion of the model and observational information, whereas the purpose of data assimilation is to reduce and control the uncertainty to achieve the optimal estimation of the entire system. As for giant, complex systems, it is very difficult to derive the probability distribution function in an analytical form; thus, eqs. (6) and (7) are usually solved with the Monte Carlo method or the ensemble method. The meaning of this approach is that every member of the ensemble is a deterministic dynamical system and the entire ensemble is a system of dynamical systems; if the members are sampled reasonably, these ensemble members can reflect the statistical characteristics of the statistical population and quantitatively characterize its uncertainty.

In addition, with consideration of the definition of observation operators, it should be highlighted that, within the framework of data assimilation, the inversion does not need to be performed independently and the radiative transfer model (along with other observation operators) only requires a forward calculation. This largely simplifies the question and eliminates the possible uncertainty caused by inversion. The data assimilation combines the forward evolution and the inversion of model state. The dynamic model is used as *a priori* information in inversion and the optimal estimation of the model state is achieved through forward iteration or recursive evolution. This is also the reason why the representativeness error of forward models was only considered in this paper.

3 Conclusions

Uncertainty is inherent to land-surface systems, and it originates in the high spatial heterogeneity of these systems. The estimation, reduction, and control of uncertainty rely on breakthroughs in the methodology and also depend on the development of new models and observational experiments that are carefully designed.

Due to ubiquitous uncertainty, the basis to estimate and control uncertainty cannot be found with deterministic ideas; instead, complex land-surface systems should be addressed from the perspective of a stochastic process, with the objects to be modeled or measured being treated as random variables. Specifically, the idea of combining dynamics and statistics is a feasible approach for modeling at macroscopic scales. This system, as commented by Weiner, is "not a single dynamic system but a statistical distribution of dynamic systems" (Wiener, 1948). As for observations, the reasonable characterization of representativeness error is a grand challenge. We should attempt to understand the uncertainty closely related to scale and design true multi-scale observations to capture spatial heterogeneity and characterize the representativeness error of observations.

The data assimilation approach is a generalized methodology to reduce and control uncertainty, and it represents a paradigm shift.

This paper does not address the following:

(1) The influence of nonlinearity is not discussed because its influence is self-evident. As shown by the equations of data assimilation, nonlinearity is a fundamental characteristic of models and observation operators, and linearity is merely a simplification of the dynamic system and measurement model.

(2) This paper does not truly discuss the scale dependence of the land surface process itself, as this question is rather complicated. If the process itself depends on the scale (such as fractal, chaos, and self-organization) (Beven, 2006; Sposito, 2008; Wheatcraft and Tyler, 1988; Young and Crawford, 2004), we must conceptualize the main characteristic scales in the models and attempt to capture these scales through observational experiments. It is desirable to systematically investigate this question in future research.

(3) One premise for controlling and reducing uncertainty is the *a priori* knowledge of uncertainty, which is true for both models and observational systems (Sun and Yeh, 2007; Neuman et al., 2010). Although this is not discussed in the present paper, it is one of the largest problems in the study of uncertainty.

In summary, the modeling and observation of landsurface systems are full of uncertainty, whereas the superposition of uncertainty does not necessarily indicate greater uncertainty. "We have the means to make a very reliable system with components that are not very reliable" (Qian, 1957). We would cite a quote from Norbert Weiner, the founder of cybernetics, to conclude this paper, "Information is information not matter or energy". The information itself is the measure of uncertainty. It can be concluded that, only when we fully use information and integrate multi-source information and apply advanced methods to address the intertwined problems of complexity, nonlinearity, uncertainty, and scale transformation, can we enhance the understanding of land-surface systems as giant, open, complex systems and ultimately improve the observability and predictability of land-surface systems.

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