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Estimating Model Parameters with Ensemble-Based Data Assimilation: Parameter Covariance Treatment

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Abstract

In this work, various methods for the estimation of the parameter uncertainty and the covariance between the parameters and the state variables are investigated using the local ensemble transform Kalman filter (LETKF). Two methods are compared for the estimation of the covariances between the state variables and the parameters: one using a single ensemble for the simultaneous estimation of model state and parameters, and the other using two separate ensembles; for the initial conditions and for the parameters. It is found that the method which uses two ensembles produces a more accurate representation of the covariances between observed variables and parameters, although this does not produce an improvement of the parameter or state estimation. The experiments show that the former method with a single ensemble is more efficient and produces results as accurate as the ones obtained with the two separate ensembles method. The impact of parameter ensemble spread upon the parameter estimation and its associated analysis is also investigated. A new approach to the optimization of the estimated parameter ensemble spread (EPES) is proposed in this work. This approach preserves the structure of the analysis error covariance matrix of the augmented state vector. Results indicate that the new approach determines the value of the parameter ensemble spread that produces the lowest errors in the analysis and in the estimated parameters. A simple low-resolution atmospheric general circulation model known as SPEEDY is used for the evaluation of the different parameter estimation techniques.

Keywords data assimilation; parameter estimation; ensemble Kalman filter; error covariance

1. Introduction

Parameter estimation using data assimilation techniques is emerging as a promising tool to constrain observationally the large set of uncertain physical parameters of current ocean and atmospheric general

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circulation models. In Ruiz et al. (2013) we presented a review of parameter estimation using ensemble based data assimilation techniques. The application of these techniques for estimating the model parameters related to a convective scheme of a simple general circulation model (GCM) was illustrated using some synthetic experiments. It was also shown that the parameter estimation has a positive impact upon the state analysis and the short to medium range forecast. The ensemble-based methods are also highly efficient with almost no extra computational cost.

The ensemble Kalman filter (EnKF) (Evensen 1994) is an advanced data assimilation method that uses the non-linear numerical model to evolve the error covariance matrix. The structure of the error covariance matrix is obtained from an ensemble of forecasts. If the state vector is augmented including model parameters, the error covariance matrix can also represent the sensitivity of the state variables to the parameters and vice versa.

Because most parameters are not directly observed, the information contained in the observations is propagated to the parameters through the error covariances between the state variables and parameters. The accuracy of the estimated parameters depends on the amount of data that contains information about the parameter value and on the accuracy of the estimated error covariances. Two different approaches have been used in the literature for estimating the covariances between the state variables and parameters: one, the so-called simultaneous approach, uses a single ensemble with perturbations in the initial conditions and model parameters, to describe the structure of the augmented state forecast error covariance matrix (Aksoy et al. 2006; Kang et al. 2011; Fertig et al. 2007; Tong and Xue 2008). The other approach known as separate approach (Koyama and Watanabe 2010) employs two separate ensembles, one for the initial conditions of the state variables and the other for the model parameters.

In the EnKF, the estimation of the uncertainty in a state variable relies on the dynamics of the system and on the information provided by observations. However, in the parameter estimation problem, the model that governs the evolution of the parameters is not known. Therefore, changes in the estimated parameters and their uncertainty are only driven by the information received from the observations. The estimation of the parameter uncertainty is a challenge for data assimilation techniques. Furthermore, stochastic parameterizations and parameter perturbations for ensemble forecasting also require some knowledge of parameter uncertainty (Posselt and Bishop 2012).

In parameter estimation applications, persistence is usually used as the model for the parameters. In this case, the ensemble spread for the estimated parameters, decrease with time and goes to zero eventually. The parameter ensemble spread will eventually became too small. To avoid this ensemble collapse, a special treatment should be applied to keep the parameter spread large enough. At the same time, the parameter ensemble spread should not be too large, because unrealistic values of the parameters can degrade the skill of the forecast (Tong and Xue 2008) producing a negative impact upon the analysis quality.

There is also another issue that affects the estimation of the parameter uncertainty in the EnKF: When the ensemble size is relatively small, sampling errors in the estimation of the covariances may artificially reduce the parameter ensemble spread even faster (Tong and Xue 2008). In this case, the spread can be reduced by more than one order of magnitude during the assimilation of observations. Once the parameter ensemble spread is too small, the observations cannot correct its value any more. In this case, this can happen before the estimated parameter gets close to its optimal value. This effect is known as filter divergence and is particularly important when global parameters (i.e., parameters which are constant over the entire model domain) are estimated without using localization, and the number of observations used in the estimation of the parameters is much larger than the size of the ensemble (Tong and Xue 2008; Koyama and Watanabe 2010).

Different approaches have been proposed in the literature to deal with this particular issue: Koyama and Watanabe (2010) use multiplicative inflation, with an inflation coefficient for the parameter ensemble different from that used for the state variables. In that work, global parameters were estimated without using localization, so that the inflation coefficient used for the parameters has to offset the above mentioned effects. Aksoy et al. (2006) propose an approach called the conditional covariance inflation (CCI) in which the parameter ensemble spread is not allowed to be smaller than a prescribed threshold. Whenever the parameter ensemble spread is smaller than the threshold, the posterior parameter ensemble perturbations are inflated back to be equal to the threshold. In practice, given that the initial parameter ensemble spread is larger than the threshold, the posterior standard deviation decreases until it reaches the threshold and then it remains constant for the following assimilation cycles (Aksoy et al. 2006). A similar approach is used by Tong and Xue (2008) but the threshold is manually tuned for each parameter individually taking into account the model sensitivity to the parameter. Zhang (2012) uses a multiplicative factor for the parameter that is computed taking into account the model sensitivity to the parameter; however, this sensitivity has to be quantified offline. Hansen and Penland (2007) use multiplicative inflation for the parameter ensemble the multiplicative inflation being selected as the minimum inflation that avoids filter divergence. Kang (2009) estimates two dimensional parameters using localization for the estimation of each local parameter. A similar approach to that proposed by Aksoy et al. (2006) is used for the estimation of the parameter ensemble spread. In addition, in this case, the inflation factor for the parameters is constrained to be smaller than the inflation applied to the state variables. This can be done because as local parameters are being estimated, the number of observations used in the estimation of each parameter is relatively small; thus the spurious reduction of the parameter ensemble spread is not present in this case and a relatively small inflation factor can keep the parameter ensemble spread large enough.

Another alternative for the representation of the parameter uncertainty and to avoid the reduction of the parameter ensemble spread, is to add some random noise to the estimated parameter ensemble to take into account model error (Ji Sun Kang, personal communication). In this case, model error arises from the fact that the estimated parameters are assumed to be constant in time, while the optimal parameter may be time-varying.

A method for the estimation of the optimal value for the parameter ensemble spread has not been provided so far. So the optimal parameter ensemble spread has to be found by computationally-expensive trial and error. The computational cost can be prohibitive if the number of estimated parameters is larger than 10. In this work, a new method to estimate the parameter ensemble spread is proposed and evaluated.

The main objective of this work is to compare the different approaches for the estimation of the components of the error covariance matrix associated to the estimated parameters in the particular case of global parameters. The different approaches are evaluated in terms of the accuracy of the estimated parameters and states using twin experiments in a perfect model scenario. This paper is organized as follows: Section 2 presents the methodology. The experiments are presented in Section 3. Section 4 describes the obtained results and conclusions are drawn in Section 5.

2. Methodology

2.1 State estimation using LETKF

To apply the LETKF method for estimating the state and model parameters, the parameters are augmented to the state vector, and the error correlations between the state variables and parameters are derived from the ensemble in the same way as the error correlations among the model state variables. As shown by Yang and DelSole (2009) the state augmentation approach can be expressed as a two-step EnKF for model parameters without direct observations, which is the case for parameters associated with model physics and numerical schemes parameters. Namely, the update for the state variables and the update for the parameters can be computed independently. This subsection describes the scheme for the state estimation. Subsection 2.2 introduces the scheme for parameter estimation.

The algorithm used in this work is the LETKF which is thoroughly described by Hunt et al. (2007). Here, only a short description of the methodology is given. The implementation is similar to that used in Miyoshi et al. (2007). This implementation has been applied to several numerical weather prediction models, including the Japan Meteorological Agency (JMA) regional and global models (Miyoshi and Aranami 2006; Miyoshi and Sato, 2007; Miyoshi et al. 2010), the AGCM for the Earth Simulator (Miyoshi and Yamane 2007) and most recently, the Weather Research and Forecasting (WRF) model (Miyoshi and Kunii 2012). The implementation of parameter estimation within the LETKF is similar to that used by Kang (2009), Kang et al. (2011), and Fertig et al. (2007), but a different localization strategy is used for the parameters.

The Kalman filter analysis equation in the LETKF is computed in the subspace spanned by the ensemble members. Following Hunt et al. (2007), the analysis ensemble mean is obtained by an optimal linear combination of the background ensemble members as follows:

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^b + \mathbf{X}^b \overline{\mathbf{w}}^a, \tag{1}$$

where $\overline{\mathbf{x}}^b$ denotes an m-dimensional vector of the background ensemble mean state, $\mathbf{X}^b$ is an $m \times k$ matrix composed of the background ensemble perturbations, and $\overline{\mathbf{w}}^a$ is a k-dimensional vector composed of the weights corresponding to the optimal linear combinations of the ensemble perturbations. Here, m and k denote the state dimension and the ensemble size, respectively. The background ensemble perturbations (i.e., the columns of the $\mathbf{X}^b$ matrix) are obtained by subtracting the background ensemble mean ($\overline{\mathbf{x}}^b$) from each of the k background ensemble members.

The optimal linear-combination weights ($\overline{\mathbf{w}}^a$) are given by

$$\overline{\mathbf{w}}^a = \tilde{\mathbf{P}}^a (\mathbf{Y}^b)^T \mathbf{R}^{-1} (\mathbf{y}^o - \overline{\mathbf{y}}^b), \tag{2}$$

where $\tilde{\mathbf{P}}^a$ is the $k \times k$ analysis error covariance matrix in the ensemble subspace (tilde indicates that the matrix lays in the ensemble subspace), $\mathbf{R}$ is the $l \times l$ observation error covariance matrix, $\mathbf{y}^o$ is the l-dimensional observation vector, and $\mathbf{Y}^b$ is an $l \times k$ matrix composed of the background ensemble perturbations in the observation space. $\overline{\mathbf{y}}^b$ is the background ensemble mean in the observation space, i.e., $\overline{\mathbf{y}}^b = \frac{1}{k}\sum_{i=1}^{k} H(\mathbf{x}^{b(i)})$, where H is the observation operator, and $\mathbf{x}^{b(i)}$ denotes the i^{th} member of the background ensemble. To compute the columns of the $\mathbf{Y}^b$ matrix, H is applied to each background ensemble member $\mathbf{x}^{b(i)}$ and the ensemble mean $\overline{\mathbf{y}}^b$ is subtracted from each member $H(\mathbf{x}^{b(i)})$ to obtain the background ensemble perturbations in the observation space.

The analysis error covariance matrix in the ensemble subspace is given by

$$\tilde{\mathbf{P}}^a = [(k-1)\mathbf{I} + (\mathbf{Y}^b)^T \mathbf{R}^{-1} \mathbf{Y}^b]^{-1}. \tag{3}$$

The analysis ensemble perturbations are obtained by

$$\mathbf{X}^a = \mathbf{X}^b \mathbf{W}^a, \tag{4}$$

where $\mathbf{W}^a$ is a weight matrix defined by

$$\mathbf{W}^a = [(k-1)\tilde{\mathbf{P}}^a]^{\frac{1}{2}}. \tag{5}$$

Localization of the background error covariance matrix for the model state variables is applied to avoid spurious error correlations between distant locations. In the LETKF, analysis is performed at each grid point independently; therefore, a very efficient parallelization is possible (Miyoshi and Yamane 2007; Miyoshi and Kunii 2012). A distance-dependent localization function is applied to the observation errors, so that distant observations have less weight (Hunt et al. 2007; Miyoshi et al. 2007; Greybush et al. 2011). Assuming that $\mathbf{R}$ is diagonal, the increase of observational error with distance is computed as follows:

$$\mathbf{R}_{l(j,j)} = \begin{cases} \mathbf{R}_{o(j,j)} \exp\left(0.5\left[\left(\frac{d_h}{d_{hs}}\right)^2 + \left(\frac{d_v}{d_{vs}}\right)^2\right]\right) & \text{if } d_h < D_h,\ d_v < D_v \\ 0 & \text{otherwise} \end{cases}$$

where $\mathbf{R}_{l(j,j)}$ is the modified diagonal element of $\mathbf{R}$ corresponding to the j^{th} observation, $\mathbf{R}_{o(j,j)}$ is the original observational error for that particular observation, d_h is the horizontal distance between the grid point in consideration and the j^{th} observation, d_v is the vertical distance, and d_{hs} and d_{vs} are the horizontal and vertical localization scales, respectively. The vertical distance is computed as the absolute value of the difference between the pressure logarithm at the analyzed grid point and the location of the observation. In this work, d_{hs} (i.e., the distance at which the observational error is increased by a factor of $\sqrt{e}$) is fixed at 700 km, and d_{vs} is fixed at 0.1. Observations farther than a certain vertical distance (D_v) or a certain horizontal distance (D_h) are omitted for the local analysis. D_v and D_h are defined by

$$D_h = 2\sqrt{\frac{10}{3}}\, d_{hs}, \tag{6}$$

$$D_v = 2\sqrt{\frac{10}{3}}\, d_{vs}, \tag{7}$$

following Miyoshi et al. (2007). Note that, as discussed in that paper, the cut-off threshold is imposed mainly to improve the computational efficiency and if its value is sufficiently large, then the discontinuity that might be introduced is small.

A common issue of the ensemble based data assimilation schemes is the lack of dispersion in the background and analysis ensembles in comparison to their actual errors. To avoid filter divergence associated with this particular issue, multiplicative inflation (Anderson and Anderson 1999) is used as in Hunt et al. (2007). The inflation parameter for the model state variables was tuned manually and set to 1.08 throughout this study.

2.2 Parameter estimation using LETKF

As stated before, when there are no direct observations of the estimated parameters, the assimilation can be split into two independent steps: one for the estimation of the state variables and the other for the estimation of the parameters. Two methods for parameter estimation are evaluated in this work: simultaneous and separate estimation.

a. Simultaneous estimation method

In the simultaneous estimation method, hereinafter referred as the simultaneous method, a single ensemble is used for the augmented state vector that contains both state variables and parameters. The model is changed slightly for each ensemble member owing to parameter evolution. The analysis ensemble mean for the parameters $\overline{\mathbf{x}}_p^a$, is given by the LETKF update:

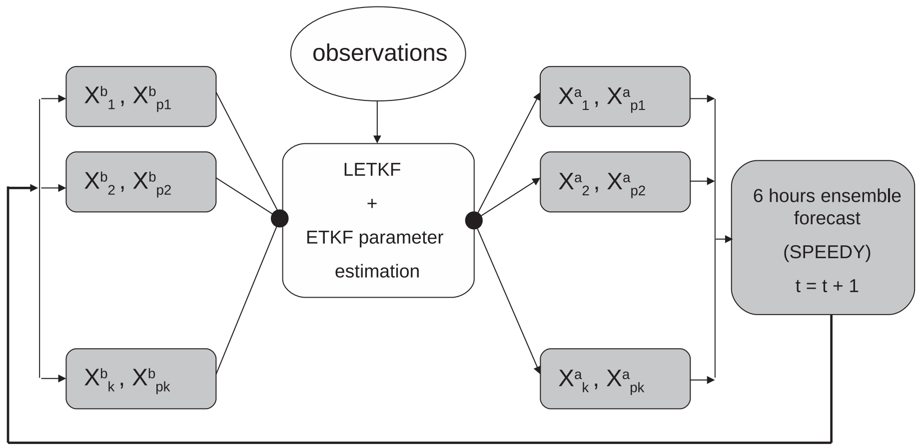

Fig. 1. Schematic representation of the initial condition and parameter estimation data assimilation cycles using the simultaneous method.

$$\overline{\mathbf{x}}_p^a = \overline{\mathbf{x}}_p^b + \mathbf{X}_p^b \overline{\mathbf{w}}^a, \tag{8}$$

where $\overline{\mathbf{x}}_p^b$ is the m_p vector of background parameter ensemble mean (with m_p the number of the estimated parameters), $\mathbf{X}_p^b$ is the $m_p \times k$ background parameter ensemble perturbation matrix. The weight vector for the parameters is obtained using (2). Note that these weights contain the information of the state variables in the observation space and the error correlation between the state variables and parameters.

The estimated parameter perturbations are obtained using

$$\mathbf{X}_p^a = \mathbf{X}_p^b \mathbf{W}^a, \tag{9}$$

where $\mathbf{W}^a$ is the transformation matrix defined in (5). The analysis covariance matrix, $\tilde{\mathbf{P}}^a$, for the parameters is calculated using the observation error covariance matrix without localization as will be discussed later. After each data assimilation step, the analyzed state and parameters are used for the next forecast. The simultaneous estimation cycle is illustrated in Fig. 1.

Individual parameter ensemble members are checked after each assimilation step to see if they remain within a realistic range defined a priori based on the physical meaning of the parameter. If the estimated parameter value for a given ensemble member is outside this range, this parameter is reverted to the physically meaningful range.

b. *Separate estimation method*

The separate estimation method, hereinafter referred as the separate method, was introduced by Koyama and Watanabe (2010). It employs two separate ensembles for the state variables and parameters. In the ensemble of state variables, only the state variables are perturbed while the parameters are not. Similarly, the other ensemble has perturbations of only the parameters. Although Koyama and Watanabe (2010) use a parameter ensemble for each member of the state-variables ensemble, in this work, a computationally cheaper variation of the method is examined. The standard LETKF assimilation (1)–(5) is performed for the model-state analysis using k ensemble members, which share the parameters from the parameter ensemble mean. The resulting analysis ensemble mean of the state variables is used as the initial condition for the parameter ensemble. The weights in (8) and (9) are computed using the ensemble with parameter perturbations. The parameter ensemble has k_p members. In general, k_p is smaller than k since the dimension of the parameter space is smaller than the state variables space. This does not remain true in the case of the estimation of the model bias where the parameter and the state space may have a similar size.

The use of the dedicated parameter ensemble in the separate method isolates the sensitivity of the system to the parameters in the hope that a more robust estimation of the optimal parameter values could be obtained. In the original implementation of Koyama and Watanabe (2010), the impact of initial condition error in the estimation of the parameters is reduced by using different state ensemble members as initial conditions for the parameter ensemble and then averaging the results. However, this approach leads to a significant increase of the computational cost as Koyama and Watanabe pointed out. The simplification

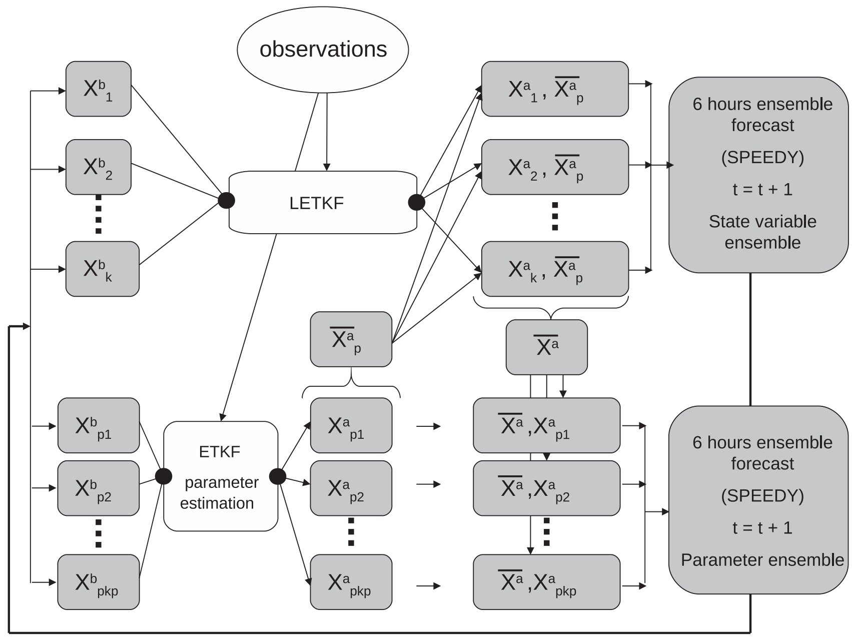

Fig. 2. Schematic representation of the initial condition and parameter estimation data assimilation cycles using the separated approach.

proposed here aims to retain the advantage of the original approach while reducing its computational cost. The current implementation is still computationally more expensive than the simultaneous method. A schematic representation of the separate parameter estimation cycle is shown in Fig. 2.

2.3 *Parameter uncertainty*

As stated before, the uncertainty of most parameters is unknown a priori. The parameter uncertainty depends not only on the model sensitivity to the parameters but also on the errors in the state variables and in the observations.

In this work, parameters are sequentially estimated as in an operational data assimilation cycle and the following three approaches are used to determine the spread of the parameter ensemble after each assimilation step. The first approach is the conditional covariance inflation (CCI) introduced by Aksoy et al. (2006) in which the parameter ensemble spread is restored to a prescribed value when it becomes smaller than the threshold. The prescribed value has to be manually tuned. The second approach is motivated by the CCI approach, the trace of the error covariance matrix for the parameters is restored to a prescribed value after the assimilation. After the update of the parameter ensemble perturbations using (9), the parameter ensemble spread is increased by factor of

$$\lambda_f = \frac{tr(\mathbf{X}_p^b \mathbf{C} \mathbf{X}_p^{bT})}{tr(\mathbf{X}_p^a \mathbf{C} \mathbf{X}_p^{aT})} \tag{10}$$

where tr stands for the trace of a matrix, $\mathbf{X}_p^b$ and $\mathbf{X}_p^a$ are the background and analysis parameter perturbations matrices of size $m_p \times k_p$. $\mathbf{C}$ is a normalization matrix that takes into account that parameters can take values which differ by several orders of magnitude. For the convective parameters used in this work, normalization is not required since the model sensitivity to these parameters is similar in magnitude, so that in this case $\mathbf{C}$ is equal to the identity matrix.

The coefficient λ_f is the same for all the parameters instead of being computed individually for each parameter as in the CCI approach. This approach will be referred to as total conditional covariance inflation (TCCI) because the total parameter space variance is restored to a time independent value (even though the spread of each individual parameter can fluctuate in time). This approach avoids the collapse of the parameter ensemble spread and also conserves the shape of the posterior parameter error covariance matrix provided by the square root filter. This is an advantage of TCCI over CCI where the posterior error covariance structure is not conserved since a different inflation factor is applied to each parameter.

Table 1. True, initial, and imperfect-model parameter values used in the experiments. The selected parameters are the inverse of the convective adjustment time scale (TRCNV), the boundary layer relative humidity threshold for convection initiation (RHBL), and the maximum lateral entrainment rate (ENTMAX).

Parameter	True value	Initial value	Imperfect-model value
TRCNV $[\mathrm{hr}^{-1}]$	0.16	0.50	0.50
RHBL [*unitless*]	0.90	0.80	0.80
ENTMAX [*unitless*]	0.50	0.30	0.30

The third method for the estimation of parameter ensemble spread is a new approach referred to as the estimated parameter ensemble spread (EPES). The weights for the parameter background ensemble perturbations $\mathbf{W}_p^a$ are multiplied by a factor

$$\lambda_e = \sqrt{\frac{k}{(k-1)tr(\tilde{\mathbf{P}}^a)}}, \tag{11}$$

note that $tr\,(\tilde{\mathbf{P}}^b) = k/(k-1)$ in the ensemble space. The updated parameter ensemble is computed using the following expression:

$$\mathbf{X}_p^a = \mathbf{X}_p^b \lambda_e \mathbf{W}^a. \tag{12}$$

With this factor λ_e the trace of the analysis error covariance matrix in the ensemble space equals the trace of the background error covariance matrix in the ensemble space. Namely, the total global ensemble spread (including both state variables and parameters) after the assimilation is assumed to be the same as the forecast ensemble spread, but preserving the structure of the analysis error covariance matrix. The inflation factor (11) is applied to the parameter perturbations only. This approach prevents the parameter ensemble spread to collapse owing to the use of a large number of observations to estimate only a small number of parameters. It also retains the structure of the analysis error covariance matrix. In particular, the relationship among the uncertainties in the different parameters is preserved as well as the relationship between the uncertainties in the parameters and in the state variables. No parameter normalization is required in this approach since the spread is computed in the ensemble subspace. This approach allows an individual evolution for the spread of each parameter and also the evolution of the total parameter ensemble spread. Note that in the data assimilation step, when parameters are estimated, no inflation is applied to the state variables. The inflation in the state variables is only used when the state estimation is performed.

3. Experiments

The experimental setting is the same as in Ruiz et al. (2013), here just a brief description is given (see Ruiz et al. (2013) for further details about the experimental setting). The SPEEDY model (Molteni 2003) is used in the experiments which is an intermediate complexity atmospheric GCM. The experiments conducted for the intercomparison of the different approaches are twin experiments in which the synthetic observations are produced with the model (Miyoshi 2005; Kang 2009; Kang et al. 2011; Fertig et al. 2009, 2007; Miyoshi 2011). The three parameters of the convective scheme of the SPEEDY model that shows the strongest sensitivity (i.e., TRCNV, RHBL, and ENTMAX) are estimated in these experiments using LETKF. As has been shown in Ruiz et al. (2013), this parameters have a strong impact upon model performance.

The parameters used in the generation of the nature or true run will be referred as the true model parameters. As in Ruiz et al. (2013), two different nature simulations are generated. One with time constant parameters equal to the default SPEEDY model parameters (Table 1) and another using temporally-varying parameters specified as follows:

$$\mathbf{x}_p(t) = \mathbf{a}\,\cos(\Omega t) + \mathrm{x}_p(0) \tag{13}$$

where $\mathbf{a}$ is the amplitude of the parameter oscillations that is different for different parameters, t is time, Ω is the frequency of parameter oscillations which is the same for each parameter and $\mathbf{x}_p(0)$ is a reference parameter set which in these experiments is equal to the set of parameters used in the constant parameter nature run (Table 1). $\Omega = \frac{2\pi}{90}\,\mathrm{day}^{-1}$ is used in the experiments. The nature simulations are generated for three months from January 1st to March 31st. The simulated observing network is the same used in Ruiz et al. (2013) and consists of regularly spaced observations located on every other model grid point and every model vertical level. Observations are available every six hours which is equal to the time between two

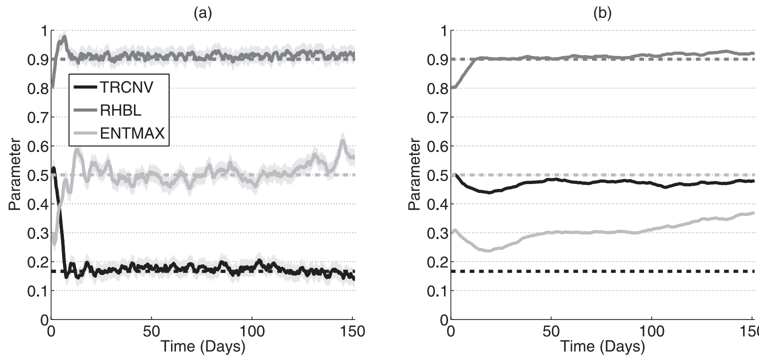

Fig. 3. Time evolution of the three estimated parameters for the simultaneous method with CCI: TRCNV, black solid line, ENTMAX, light grey solid line, and RHBL, dark grey solid line. The shade around the estimated parameter indicates the ensemble spread (± one parameter ensemble perturbation spread). The true parameter values are also indicated: TRCNV, black dashed line, ENTMAX, light grey dashed line, and RHBL dark grey dashed line. Panel (a) shows the results for the experiment with an initial parameter ensemble spread of 2.9×10^{-2} and panel (b) the results for the experiment with an initial ensemble spread of 2.9×10^{-3}. In both cases the true parameters are constant in time.

assimilations.

The model used in the data assimilation cycle is the same as the one used in the nature runs, except the parameters in the nature simulations are set to the true values while the parameters in the data assimilation cycle are being estimated. This implies that although the model used in the data assimilation system is imperfect, the imperfection is purely due to the imperfect values of the three model parameters.

The initial parameter values for the first cycle are different from the true values, as shown in the "initial value" column of Table 1. The value of different parameters, with different units, cannot be directly compared. Therefore, in this work, parameters are scaled by the width of their physically meaningful range. This width is set to 1 hr^{-1} for TRCNV and to 1 for the non-dimensional parameters ENTMAX and RHBL. Hereafter, all the values expressed in the text corresponds to the normalized non-dimensional parameter values.

4. Results

Two sets of experiments are examined. First, one set of experiments explores the sensitivity to parameter ensemble spread using the approaches introduced in Section 2.3. Second, experiments comparing the two methods of parameter estimation, simultaneous method, and separate method, are analyzed.

4.1 *Comparison of parameter spread computation approaches*

The experiments in this section compare the three approaches for parameter ensemble spread computation, the CCI, TCCI and EPES as defined in Section 2.3. They are based on the simultaneous method for the estimation of the state and the parameters with an ensemble size of 20 members and an assimilation window length of six hours. For each approach, 15 assimilation experiments were conducted with an initial ensemble spread between 2.5×10^{-3} and 2.0×10^{-1} logarithmically spaced. Manual tuning of the parameter ensemble spread suggests that the optimum spread value is around 2.5×10^{-2}, thus the selected range contains the optimal value. At the beginning of each data assimilation experiment, the same value is assigned to the spread of each parameter. The parameter perturbations are randomly generated assuming a normal distribution with no correlations among the different parameters.

Figure 3a shows the estimated parameter evolution using the CCI approach for temporally fixed parameters. The initial parameter ensemble spread is 2.9×10^{-2}. As has been discussed in Ruiz et al. (2013), the estimated parameters converge to the true parameter value in less than 20 days; after that, the estimated parameters oscillate around the true value. This oscillation might be mostly associated with the uncertainty coming from errors in state and in observations. The results are quite sensitive to the initial parameter ensemble spread. If the initial ensemble spread is set to 2.9×10^{-3} (Fig. 3b), two of the three parameters fail to converge to their true values. Note that TRCNV (black solid line) is close to the ENTMAX true value is 0.5, instead of its true value

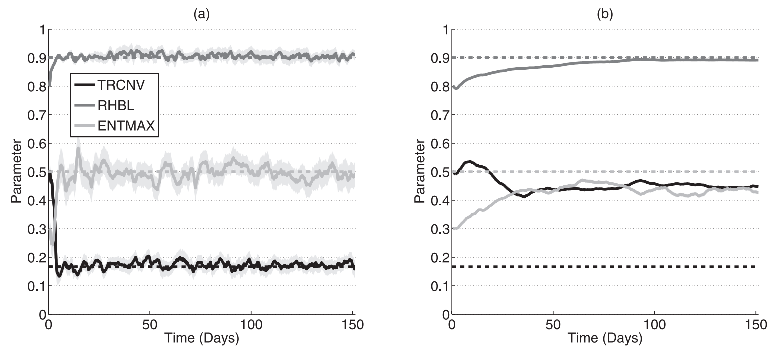

Fig. 4. As in Fig. 3, but for the TCCI approach.

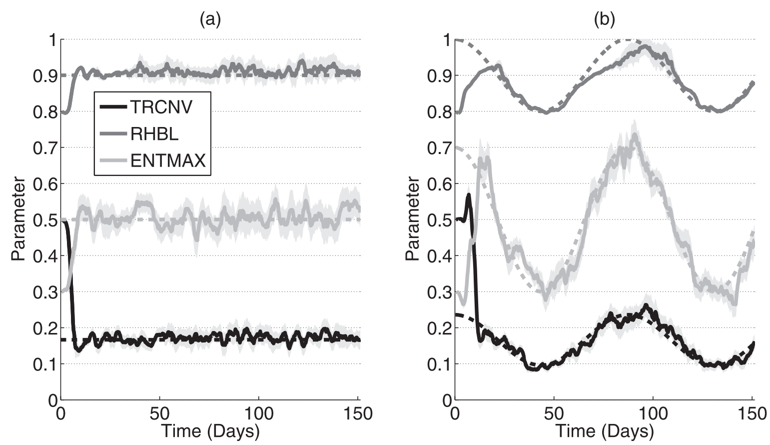

Fig. 5. Time evolution of the three estimated parameters for the simultaneous method with EPES: TRCNV, black solid line, ENTMAX, light grey solid line, and RHBL, dark grey solid line. The shade around the estimated parameter indicates the ensemble spread ($\pm$ one parameter ensemble perturbation spread). The true parameter values evolution are also indicated: TRCNV, black dashed line, ENTMAX, light grey dashed line, and RHBL, dark grey dashed line. Panel (a) shows the results for the experiment with an initial parameter ensemble spread of 2.9×10^{-3} and panel (b), as in (a), but for the time dependent parameters. In both cases the true parameters are constant in time.

which is 0.16. Therefore, a conclusion of the experiments is that the initial ensemble spread for the CCI approach has to be manually tuned to obtain a good estimation of the parameters. A similar sensitivity of the estimated parameters to the initial ensemble spread when CCI is used is obtained when the true parameters are time dependent (not shown).

Figure 4 shows the estimated parameter evolution using the TCCI approach. Results are similar to the ones obtained with CCI. The ensemble spread varies with time among the different parameters (Fig. 4a) even when the total spread associated with the parameters is fixed in time. Those parameters associated with a stronger model sensitivity have lower spread. This is consistent with the idea that the parameters with stronger model sensitivity can be more efficiently constrained by the observations. This shows that the structure of the analysis error covariance matrix for the parameters as estimated with the ensemble square root filter has valuable information about the model sensitivity to the parameter and that this information should be taken into account. As in the CCI experiment, when the total parameter ensemble spread is too small, the estimated parameters do not converge to their true values (Fig. 4b).

Figure 5 shows the evolution of the estimated parameters using the novel approach, EPES, that is proposed in this work. Figure 5a shows the estimated

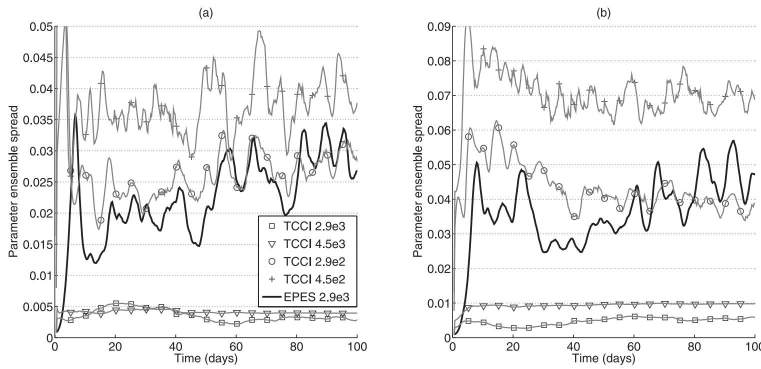

Fig. 6. Parameter ensemble spread for the EPES approach as a function of time for the 2.9×10^{-3} initial parameter ensemble spread (black tick line) and for the TCCI approach for different initial parameter ensemble spreads: 2.9×10^{-3} (grey line with squares), 4.5×10^{-3} (grey line with triangles), 2.9×10^{-2} (grey line with circles), and 4.5×10^{-2} (grey line with crosses), (a) TRCNV and (b) ENTMAX.

parameters using the same initial ensemble spread that produces the failure in the estimation of the parameters using CCI and TCCI approaches. As in the TCCI case, the parameter ensemble spread of each parameter changes with time, and it is different for each estimated parameter. Figure 5b shows the estimated parameter evolution for time-varying parameters using EPES. The technique can adequately capture the evolution of the parameters. However, even when the frequency of the parameter oscillation is low, there is a small temporal lag between the estimated parameters and their true evolution. Similar results (not shown) are obtained with the CCI and TCCI approaches when the parameter ensemble spread is properly tuned.

As can be seen in Fig. 5b, the EPES approach can efficiently detect changes in the model sensitivity to the parameters and it can modify the parameter ensemble spread according to those changes. For instance, the spread associated with RHBL changes with time in the time-dependent parameter experiment. As has been shown in Ruiz et al. (2013) (in Fig. 1), when the true parameter is lower than 0.9, the sensitivity to this parameter is strong and consistently the estimated parameter ensemble spread is low. In contrast, when the true parameter is over 0.9, the model is almost insensitive to changes in this parameter and the estimated ensemble spread for this parameter increases. A similar behavior is obtained for the TRCNV parameter, which also shows some asymmetries in the model sensitivity to the parameter. For the ENTMAX parameter, the cost function of the parameter is symmetric and so the parameter ensemble spread is almost the same independently of the value of the estimated parameter.

The evolution of the parameter ensemble spread by the TCCI and the EPES for 4 selected initial parameter ensemble spread values is shown in Fig. 6. Both methods can adequately capture the differences in the parameter ensemble spread for the different parameters consistently with the model sensitivity to each parameter (compare Figs. 6a and 6b). The spread of TRCNV parameter is almost half of the spread of ENTMAX in almost all the experiments presented in the figure. This is because model sensitivity to ENTMAX is much weaker. In the case of the TCCI approach, the parameter ensemble spread depends on its initial value because the sum of the ensemble spreads of the three parameters is fixed in time. In the case of the EPES approach, the parameter ensemble spread is independent of the initial value and only the experiment starting with the lowest parameter ensemble spread is shown. In this experiment, the parameter ensemble spread rapidly increases with time during the first data assimilation cycles, and converges to the total parameter spread of approximately 2.5×10^{-2}. The experiments that used the EPES approach converge to the same value independently of the initial parameter ensemble spread (not shown). This value is a measure of the uncertainty of the estimated parameter given the available information.

The impact of the different approaches for the computation of the parameter ensemble spread on the error in the state variables is examined. The analysis error for the state variables is computed using a root mean squared error (RMSE) weighted by the inverse of the observational error:

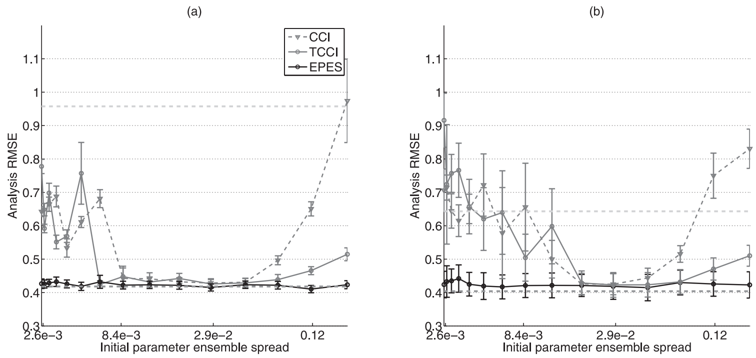

Fig. 7. Time-averaged analysis RMSE as a function of initial parameter ensemble spread for the simultaneous method with the EPES (black line), TCCI (grey dashed line), and CCI (grey solid line) approaches. The time-averaged RMSE corresponding to the perfect model (grey dashed line) and to the imperfect model (light grey dashed line) are also included. Constant true parameters experiments (a) and time-varying true parameters (b).

$$RMSE = \sqrt{\frac{1}{N}(\overline{\mathbf{x}}^a - \overline{\mathbf{x}}^t)^T A^{-1} (\overline{\mathbf{x}}^a - \overline{\mathbf{x}}^t)}\,. \tag{14}$$

Where A defines the norm and is a diagonal matrix of size $N \times N$ which contains the typical error magnitudes of each state variable. The typical error magnitudes are chosen to be equal to the observational errors of each variable. Only the model state variables are considered for the computation of the analysis RMSE. The time averaging is computed using the last 200 cycles (≈ 50 days) to assure that convergence has been reached. A perfect model experiment (i.e., a data assimilation cycle using the true parameter values) and an imperfect model experiment were also performed. For the constant parameter case, the imperfect model experiment consists of a data assimilation cycle using the model with an incorrect set of parameters as shown in Table 1. In the case of the time-varying parameters, the imperfect model consists of a data assimilation cycle which uses the time average of the true time-varying parameters. In this case, the imperfect model does not take into account the time variability of the true parameters; however, the selected value for the parameters is one of the most reasonable choices that can be done.

Figure 7a shows the time-averaged analysis RMSE for the experiments using the CCI, TCCI, and EPES approaches for the experiment with time-independent true parameters. The analysis error corresponding to the parameter estimation experiments is close to the analysis error of the perfect model for most of the experiments. This shows that the parameter estimation is successful in terms of finding the optimal parameter value and in terms of the reduction of analysis error associated with model error. For the CCI and TCCI approaches, the RMSE is larger for non-optimal initial parameter ensemble spread. This is due to two main reasons: Larger parameter ensemble spreads produce an increase in the parameter estimation noise that degrade the analysis. Moreover, for the two largest parameter ensemble spreads, estimated parameters of some ensemble members usually fall outside the prescribed range for the parameters. In these cases, the estimated parameter values are forced back to the prescribed range and the order and the mean of the parameter ensemble are not preserved, thus degrading the estimation. On the other hand, if the parameter ensemble spread is too small, it will result in the lack of convergence in the parameters (or a convergence rate that is too slow). The RMSE is minimum for a range of initial parameter spread values which is almost the same for both methods. Away from this range, RMSE values are lower for the TCCI approach compared to CCI indicating that taking into account the relationship among the uncertainty in the different parameters produces a positive impact in the analysis.

In the case of the EPES approach, the analysis RMSE is almost independent of the initial parameter ensemble spread. The EPES RMSE is lower than the RMSE for the CCI and TCCI approaches for almost all of the initial parameter ensemble spread values. This shows that the estimated ensemble spread approach not only converges to the same value of parameter ensemble spread independently of the initial ensemble spread, but also it converges to the value that produces the lowest analysis error at almost no additional computational cost. This shows that the augmented state analysis error covariance matrix obtained with the

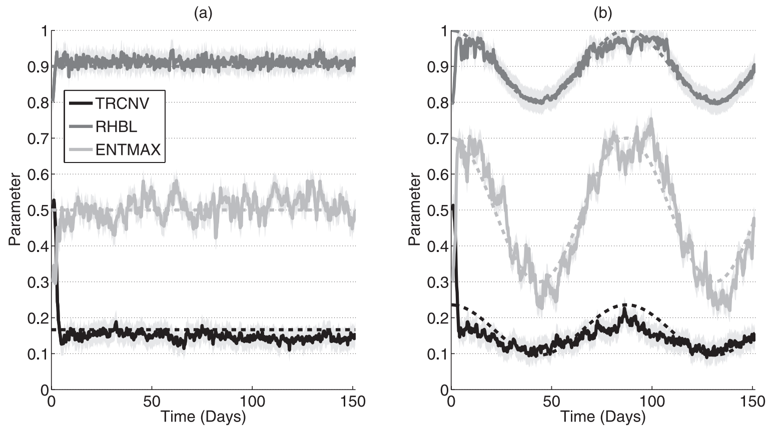

Fig. 8. As in Fig. 5, but for the parallel method and the CCI approach.

ensemble transform Kalman filter has information about the relative magnitude of the spread in the state variables and in the parameters as well as among the parameters. This information should be used, as in this case, to estimate the parameter uncertainty.

Similar results are found in the case of time-dependent parameters Fig. 7b. In this experiment, the difference between the perfect and imperfect model experiment can be interpreted as the impact of not taking into account the time dependence of the model parameters. A difference of the time-varying parameters with respect to the constant parameters is that independently of the parameter ensemble spread approach, the analysis error in the parameter estimation experiments are slightly higher than in the perfect model case. This is probably because the nature run is evolved with a model with smooth time-varying parameters, although the parameters used in the forecast model of the assimilation system are assumed to be constant within the assimilation window the estimated parameters change abruptly at the assimilation times, producing a piecewise-constant time variation of the estimated parameters. In the case of the time-varying parameters once again EPES approach produces the lowest RMSE for all the initial ensemble spread values; the CCI and TCCI approaches produce low RMSE values for a narrow initial spread range.

4.2 Comparison of the simultaneous and separate methods

The data assimilation experiments using different initial parameter ensemble spreads are repeated using the separate method. The CCI approach is used in this case. The sizes of the state ensemble and parameter ensemble are chosen to be 20 and 5 members, respectively. Preliminary tests showed that 5 members are sufficient to obtain an accurate estimation of the parameters. Note that there are only three free parameters.

Figure 8a shows the evolution of the estimated parameters with an initial ensemble spread of 2.5×10^{-2} using the separate method for the case of a constant true parameter. The separate method can find the correct value for the RHBL and ENTMAX parameters. However, the TRCNV parameter is not estimated correctly. The reason for the small bias in the estimation is not clear, but as will be shown, this bias has almost no effect upon the analysis quality. For the time-varying parameter experiment, the separate method provides good estimates for the parameter RHBL (Fig. 8b). However, there is an underestimation of the amplitude of the oscillation in TRCNV and an overestimation of the amplitude in the oscillation of ENTMAX.

In the separate method (Fig. 8), the estimated parameters show a higher frequency variability than in the simultaneous method (Fig. 5). One possible reason is that in the case of the simultaneous method, noise in the parameter estimation may be connected to relatively low-frequency errors in the state variables. In fact, the RMSE of the individual ensemble members in the simultaneous method shows oscillations that have similar frequencies to those found in the estimated parameter (not shown). The low-frequency error in the state variables is also present in the perfect model experiment in which no parameter estimation is performed. This effect is not present in the separate method since all parameter ensemble members start

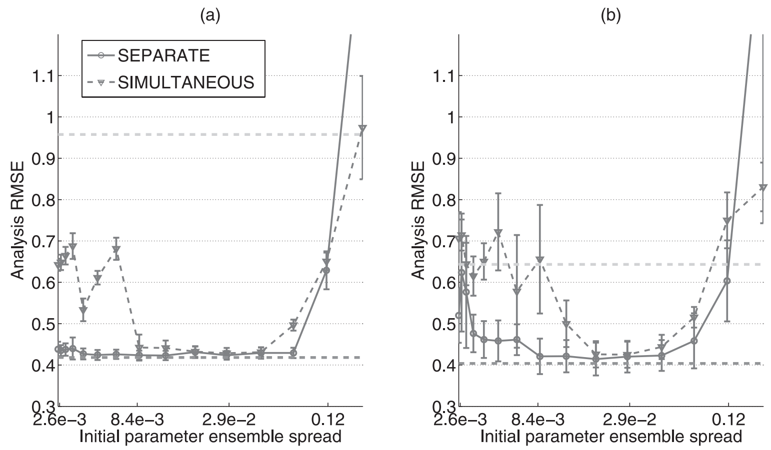

Fig. 9. RMSE of the analysis as a function of the initial ensemble spread using the CCI approach and the simultaneous method (black line) and the separate method (grey line). Panel (a) shows the results for the constant true parameter experiment and panel (b) shows the results for the time-dependent true parameter experiment. The time-averaged RMSE corresponding to the perfect model (grey dashed line) and to the imperfect model (light grey dashed line) are also included.

from the same initial state and thus the estimation error might be dominated by random errors in the observations.

The RMSE for different initial spreads using the separate method is shown in Fig. 9. The separate method achieves its lowest analysis RMSE for smaller initial parameter ensemble spread values. The sensitivity of the analysis RMSE to the initial ensemble spread is also weaker for this method. This might be because the sensitivity of the model to the parameters is isolated from the sensitivity to the initial conditions in the case of the separate method. Under these conditions, LETKF can obtain the correct value for the parameters even when the impact of the parameter perturbations is much smaller than the sensitivity to the initial condition perturbations. This can explain why even for the lowest initial parameter ensemble spread the separate method is successful in estimating the parameters while the simultaneous method, using CCI parameter spread approach, fails. The minimum RMSE obtained with the separate and the simultaneous methods are almost the same.

To further explore how the separate and simultaneous method represent the covariances between errors in the parameters and errors in the state variables, these covariances are explicitly computed from the ensemble for all the variables and for the full length of the experiment. Figure 10 shows the covariance between the specific humidity and the TRCNV parameter for the lowest model level and for the 300^{th} assimilation cycle. Figure 10a, generally shows negative covariance between TRCNV and specific humidity near the surface. As TRCNV increases, the strength of the parametrized convection increases and more moisture is transported upward from the boundary layer. Then, the specific humidity in the lowest model level decreases. In the separate method, there is a strong spatial correlation between the regions where convection is active and the regions where the correlation between TRCNV and low-level moisture is strong. This covariance is physically consistent with the expected sensitivity of the model to changes in this parameter as discussed above.

In the case of the simultaneous method (Fig. 10b), the spatial distribution of the covariance between TRCNV and low-level moisture in the model is noisier. The physically consistent pattern is still present, however, there are also regions where the covariances are relatively large and no precipitation is present. The noise comes from the perturbations in the initial conditions that produce spurious covariances between the parameter and the state variables.

Figure 11 shows the covariances for the 300^{th} assimilation cycle between the wind components at upper levels and the TRCNV parameter. For the separate method, a higher TRCNV value, which is associated with stronger convection, produces enhanced upper level divergence. This is expected since stronger heating at middle levels associated with convection will produce large-scale upward motion

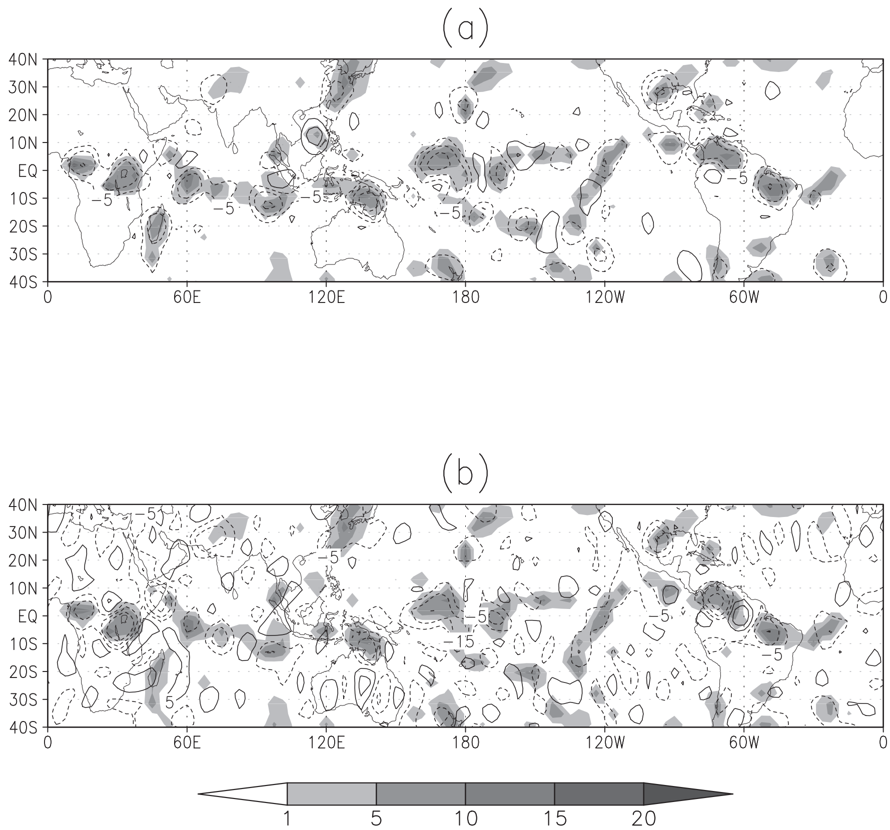

Fig. 10. Forecasted 6 h total accumulated precipitation (mm, shaded) and covariance between the TRCNV parameter and the specific humidity at the lowest model level (1×10^{-7}. Panel (a) shows the results for the separate method and (b) for the simultaneous method. Both panels corresponds to the 300^{th} assimilation cycle.

and divergence at upper levels. In the simultaneous method, the noise associated with the initial condition perturbations in the wind field is greater than the sensitivity of the wind to the convective scheme parameters, so that finding the enhanced divergence in convective areas is not considerably easy. This confirms that the separate method isolates better the physically consistent covariances between the parameters and the state variables. This corroborates that the separate method is able to capture the model sensitivity to changes in the parameters even when this sensitivity is small compared to the errors in the initial conditions as has been previously shown in this section.

In the experiments shown thus far, the simultaneous method may be advantageous because it provides an unbiased estimation of the parameters. Furthermore, EPES parameter ensemble spread approach can be used in the simultaneous method which gives stable performance independently of the initial parameter ensemble spread. The computational cost of the two methods are also different. The simultaneous method uses essentially the same amount of resources as a standard data assimilation cycle based on the LETKF, since the estimation of global parameters is computationally cheap when the estimation is performed in the ensemble space. In contrast, the separate method requires more model simulations to construct the ensemble of parameter perturbations.

To compare the two methods considering the computational cost, three assimilation cycles of the two methods with the same number of model integrations were conducted, in which the ensemble sizes were of 25, 45, and 65 members. The size of the parameter ensemble in the separate method is always set to 5 members as in the previous experiments, and only the size of the state ensemble is changed. For instance, the separate method in the 25-member experiment uses an ensemble of 20 members for the state estimation and a 5 member ensemble for the parameter estimation, while the simultaneous method

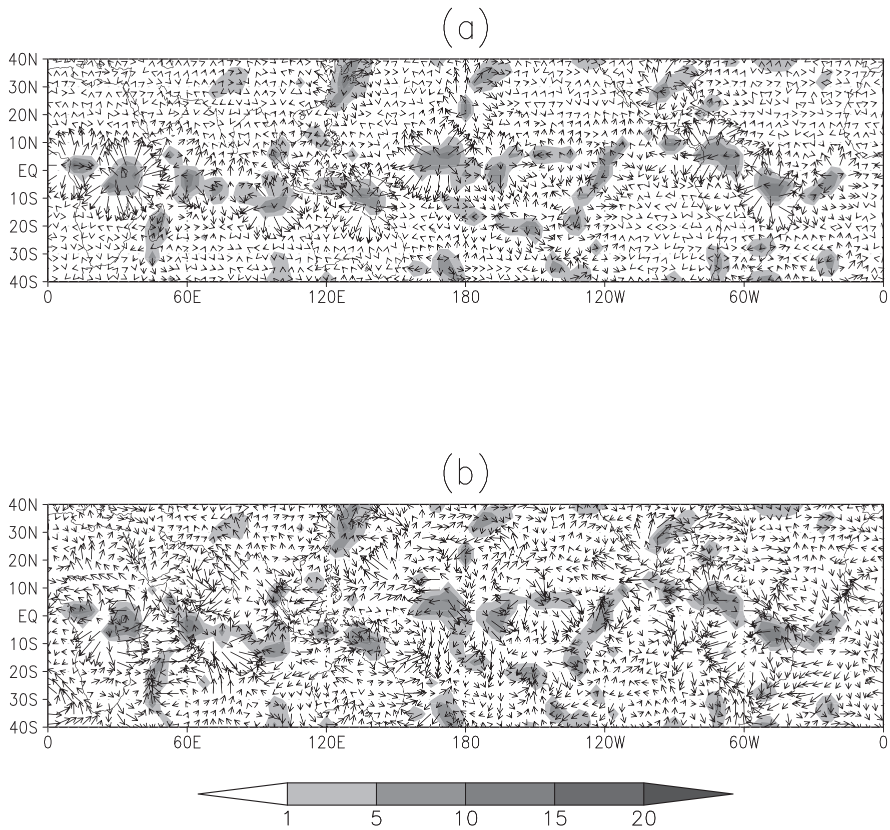

Fig. 11. Forecasted 6 h total accumulated precipitation (mm, shaded) and covariance between the TRCNV parameter and the wind components at the top of the troposphere (vectors). Panel (a) shows the results for the separate method and (b) for the simultaneous method. Both panels correspond to the 300^{th} assimilation cycle.

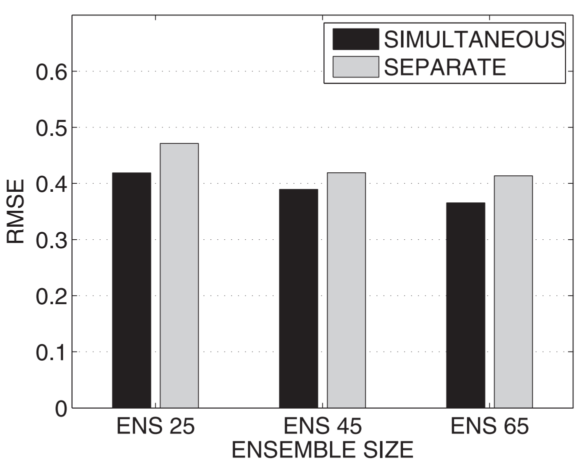

Fig. 12. Time-averaged analysis RMSE for the data assimilation experiments performed using three different ensemble sizes. The black bars correspond to the simultaneous method and the grey bars to the separate method.

uses an ensemble of 25 members for the augmented state estimation. The CCI with an initial spread of 2.5×10^{-2} is used in all cases. Figure 12 shows that the analysis RMSE decreases with ensemble size as expected for both parameter estimation methods. For all cases, the simultaneous method produces better results for the same ensemble size. Furthermore, the impact of increasing the ensemble size from 45 to 65 is larger for the simultaneous method.

5. Conclusions

In this work, the sensitivity of the parameter estimation to the accuracy of the estimation of the parameter ensemble spread and the covariances between the parameter and the state variables were explored. A new approach was introduced and evaluated for the estimation of the optimal parameter ensemble spread. The new EPES approach produced a significant improvement in the parameter estimation. When parameters were time-dependent the model sensitivity to the parameters could also change with time. In this case, the EPES approach was able to capture changes in the strength of the model sensitivity to the parameters adapting the parameter ensemble spread to the sensitivity level. The EPES approach also avoided filter divergence even when a large number of observations is used to estimate global parameters without using localization and with a limited ensemble size. Moreover, this approach provided an estimation of the parameter uncertainty that can be used to generate optimal parameter perturbations to account for model uncertainty in ensemble forecasting. This estimation of the parameter uncertainty might be also used as a criterion for parameter identifiability. If the estimated uncertainty is larger than the physically meaningful range of the parameter, this might indicate that the parameter is not identifiable, i.e., it cannot be estimated on the basis of the available information.

The EPES approach uses the information contained in the analysis error covariance matrix of the augmented state. In the LETKF method, perturbations for the parameters and for the state variables are constructed using a square-root filter method. In this work, we found that the EPES approach provides a good estimation of the relative magnitude of the spread of the different parameters. The relative spread magnitude was also consistent with the sensitivity of the model to the parameters.

The application of EPES approach appears to be promising for estimating on-line parameters augmented to the model state in general circulation models using LETKF method. In this work, the EPES approach is applied to the estimation of global parameters in the general circulation model with no spatial localization in a perfect model scenario. The performance of the EPES approach in this scenario is better and more robust compare with CCI and TCCI approaches. However, it is not clear whether EPES approach will still be successfull under more realistic scenarios, such as the estimation of 2 or 3 dimensional parameters or in the case of an imperfect model. Future work will focus on determining whether the EPES approach can find the optimal parameter ensemble spread under more realistic conditions.

This study also evaluated two different methods: the simultaneous method and separate method. The separate method permitted a better isolation of the sensitivity of the model state to changes in the parameter. However, the simultaneous method produced similar results in terms of the analysis RMSE and it produced marginally better results in terms of the error in the estimated parameters. Moreover, the separate method required additional model integrations compared with a standard assimilation cycle (without parameter estimation) while the simultaneous method did not. Both methods only required minor changes in the model and the assimilation system codes. When the extra computational effort required by the separate method was used to increase the number of ensemble members in the simultaneous method, the analysis error was reduced more effectively. These results suggest that among the different implementations tested in this work, the simultaneous method with the proposed EPES approach produced the best results at low extra computational cost compared with the cost of a standard assimilation system. Although in the experiments presented in this work, the simultaneous approach shows some advantages, the separate method seems to be more robust when the sensitivity of the model to the parameters is weak, i.e., in cases where the parameter is less identifiable. This suggests that the separate method may be advantageous in other parameter estimation applications. Additional work is needed to compare these techniques for the estimation of two and three dimensional parameters and in cases where the number of available observations is not as high as in this case.

In the experiments presented in this work, the model imperfections were directly related to the uncertainty in the value of the convective scheme parameters. In real-world applications, the sources of model error are diverse; such as different parameterizations and limited resolution. Future work will focus on parameter estimation with different sources of model error to examine if the technique reduces model error even when the estimated parameters cannot explain all model error sources. Another important issue to be addressed is whether an optimal spatial distribution for the parameters can be obtained. Promising results have been obtained in Kang (2009) for CO_2 flux sources. Spatio-temporally dependent parameters could lead to an improvement of model performance as well as to a better understanding of the underlying physical processes.

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