Non-Gaussian Probability Densities of Convection Initiation and Development Investigated Using a Particle Filter with a Storm-Scale Numerical Weather Prediction Model

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ABSTRACT

Non-Gaussian probability density functions (PDFs) in convection initiation (CI) and development were investigated using a particle filter with a storm-scale numerical prediction model and an adaptive observation error estimator (NHM-RPF). An observing system simulation experiment (OSSE) was conducted with a 90-min assimilation period and 1000 particles at a 2-km grid spacing. Pseudosurface observations of potential temperature (PT), winds, water vapor (QV), and pseudoradar observations of rainwater (QR) in the lower troposphere were created in a nature run that simulated a well-developed cumulonimbus. The results of the OSSE (PF) show a significant improvement in comparison to ensemble simulations without any observations. The Gaussianity of the PDFs for PF in the CI area was evaluated using the Bayesian information criterion to compare goodness-of-fit of Gaussian, two-Gaussian mixture, and histogram models. The PDFs are strongly non-Gaussian when NHM-RPF produces diverse particles over the CI period. The non-Gaussian PDF of the updraft is followed by the upper-bounded PDF of the relative humidity, which produces non-Gaussian PDFs of QV and PT. The PDFs of the cloud water and QR are strongly non-Gaussian throughout the experimental period. We conclude that the non-Gaussianity of the CI originated from the non-Gaussianity of the updraft. In addition, we show that the adaptive observation error estimator significantly contributes to the stability of PF and the robustness to many observations.

1. Introduction

Among the great challenges in meteorology is understanding and then predicting the initiation and development of severe mesoscale convective systems (MCSs). These systems generate lightning, downbursts, tornados, and flash floods that often cause human casualties as well as property damage and economic losses, particularly in urban areas. The difficulty in understanding and predicting MCSs stems from their small scale in terms of both time [$O(1)$ h] and space [$O(10)$ km] as well as their strong nonlinearity (e.g., Sun et al. 2014; Yano et al. 2018). Thus, to investigate MCS mechanisms, it is

necessary to use remote sensing observations, numerical weather prediction (NWP) model simulations with data assimilation (DA), and ensemble prediction. Several successful field campaigns that have been conducted, such as the Convective and Orographically induced Precipitation Study (COPS; Wulfmeyer et al. 2011), Tokyo Metropolitan Area Convection Study for Extreme Weather Resilient Cities (TOMACS; Misumi et al. 2019), and Plains Elevated Convection At Night (PECAN) field campaign (Geerts et al. 2017), have indicated that abundant observations can improve NWP skills through DA. In fact, many studies have used advanced DA techniques to successfully predict small-scale MCSs and investigate their mechanisms (e.g., Aksoy et al. 2010; Yussouf et al. 2013).

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For instance, [Kawabata et al. \(2007\)](#) successfully predicted a small and isolated MCS before initiation with accurate intensity and timing using a storm-scale, four-dimensional, variational DA system, while [Yokota et al. \(2018\)](#) identified important factors of supercell tornado genesis using an ensemble Kalman filter (EnKF).

However, because the atmosphere is quite sensitive to small, initial state perturbations, it shows behaviors referred to as “chaotic” ([Lorenz 1969](#)); MCSs, in particular, can be described as highly chaotic. [Zhang et al. \(2003\)](#) investigated the intrinsic predictability in meso-scale prediction by comparing perturbed and non-perturbed predictions between dry and moist models. They concluded that the parameterization of moist convection itself in a numerical model limits the predictability of mesoscale predictions. Their conclusion results in a certain speculation that the moist processes in numerical models are strongly nonlinear and thus chaotic.

Nonlinearity in moist processes leads to non-Gaussian statistics of precipitation in both observations and NWP model outputs. This is quite problematic for DA because most DA theories, such as the variational and Kalman filter methods, assume linear processes of numerical models and observational operators and Gaussian probability density functions (PDFs) in errors of numerical models and observations (e.g., [Kalnay 2002](#)). For the successful assimilation of precipitation data, special treatments are needed to address non-Gaussianity. [Koizumi et al. \(2005\)](#) found that errors of precipitation in an NWP model follow an exponential distribution. They proposed a special statistical model for assimilating precipitation data in a variational framework. To address non-Gaussianity in precipitation assimilations, [Lien et al. \(2013\)](#) proposed a Gaussian transformation of precipitation data in an intermediate atmospheric general circulation model (AGCM) and obtained a promising result. [Kotsuki et al. \(2017\)](#) applied their method to the assimilation of satellite-derived precipitation data with a global nonhydrostatic model and succeeded in improving the precipitation forecast skill.

Nonlinearity in the atmosphere and non-Gaussianity of the PDFs make it difficult to investigate severe MCSs using NWP models. [Miyoshi et al. \(2014\)](#) and [Kondo and Miyoshi \(2016\)](#) conducted an EnKF experiment with 10240 members using an AGCM and found non-Gaussian PDFs of specific humidity in the modeled atmosphere that were likely related to moist convection. Because a Gaussian-based EnKF cannot adequately represent and maintain such non-Gaussian PDFs in the ensemble, it is difficult to use EnKF systems to investigate such phenomena.

A particle filter is an excellent choice for addressing this difficulty and investigating CI because it explicitly addresses the nonlinearity that leads to non-Gaussian PDFs (e.g., [van Leeuwen 2009](#)). Furthermore, because no assumption is made on prior and posterior PDFs of ensemble members, a particle filter can be used to sample Gaussian as well as non-Gaussian PDFs in the ensemble that are thought to be closely related to moist convection. Given the aforementioned issues we sought to answer the following question: what is the source of the chaos in MCSs?

[Poterjoy et al. \(2017\)](#) pioneered the application of a particle filter to convective-scale DA. They implemented a localized particle filter ([Poterjoy 2016](#)) in the Weather Research and Forecasting Model ([Skamarock et al. 2008](#)) and conducted an observing system simulation experiment (OSSE) to assimilate pseudoradar data. They compared the OSSE results to those of EnKF assimilation and found that the probability distributions of the hydrometers in a well-developed MCS were implausible in the EnKF assimilation. However, the particle filter more accurately captured the distributions because of its ability to address the non-Gaussianity. This result motivated us to investigate PDFs on CI and development using a particle filter with a nonhydrostatic model.

Among the difficulties for particle filters is “filter collapse,” whereby one particle receives all the weight. Thus, large ensemble sizes are required up to the degrees of freedom observed by measurements and the accuracy of these measurements ([Bickel et al. 2008](#); [Bengtsson et al. 2008](#); [Snyder et al. 2008](#)). To address this problem, [Poterjoy \(2016\)](#) and [Potthast et al. \(2019\)](#) developed localized particle filters that limit available observations in space at filtering step. In this manuscript, we propose a particle filter with an adaptive observation error estimator ([Ueno and Nakamura 2016](#)) to mitigate the filter collapse.

In this paper, the particle filter DA is described in [section 2](#) and the OSSE performed with the filter is described and examined in [section 3](#). The PDFs related to CI and development, effects of adaptive estimation of observation errors, and the number of observations are discussed in [section 4](#). A summary and conclusions are presented in [section 5](#).

2. NHM-RPF

The particle filter consists of two parts: a time-integration numerical model and a filtering model. For the numerical model, we adopted the Japan Meteorological Agency (JMA) nonhydrostatic model (JMANHM; [Saito et al. 2006, 2007](#); [Saito 2012](#)). This model

was used as the operational mesoscale model at the JMA until 2017 and it implements various physical processes, including four-ice and two-moment cloud microphysics, and the Deardorff turbulence scheme (Deardorff 1980).

The filtering model is based on Bayes's theory as follows:

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{x})p(\mathbf{y}|\mathbf{x})}{\int p(\mathbf{y}|\mathbf{x})p(\mathbf{x})d\mathbf{x}}, \quad (1)$$

where $p(\mathbf{x})$ is the prior PDF of the modeled atmosphere $\mathbf{x}$, $p(\mathbf{y}|\mathbf{x})$ is the likelihood of observation $\mathbf{y}$, and $p(\mathbf{x}|\mathbf{y})$ is the posterior PDF; the denominator on the right-hand side of Eq. (1) works as a normalization factor. In the present study, the likelihood $p(\mathbf{y}|\mathbf{x})$ is assumed to be Gaussian as follows:

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{\sqrt{2\pi|\mathbf{R}|}} \exp\left\{-\frac{1}{2}[\mathbf{y} - H(\mathbf{x})]^T \mathbf{R}^{-1}[\mathbf{y} - H(\mathbf{x})]\right\}, \quad (2)$$

where, $\mathbf{R}$, $|\cdot|$, and H denote observational error covariance, determinant, and observational operators, respectively.

To obtain $p(\mathbf{x}|\mathbf{y})$, we introduce a Monte Carlo approximation of $p(\mathbf{x})$, in which the prior PDF is discretized by N particles with delta functions, as follows:

$$p(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i), \quad (3)$$

where N is the ensemble size, i is an individual ensemble member, and $\mathbf{x}_i$ is a prognostic variable in the ensemble member. The posterior PDF is then discretized as follows:

$$p(\mathbf{x}|\mathbf{y}) = \sum_{i=1}^N w_i \delta(\mathbf{x} - \mathbf{x}_i), \quad (4)$$

with the weight w_i given by the following:

$$w_i = \frac{p(\mathbf{y}|\mathbf{x}_i)}{\sum_{i=1}^N p(\mathbf{y}|\mathbf{x}_i)}. \quad (5)$$

The effective sample size (ESS; Reich and Cotter 2015) is given by the following:

$$M_e = \frac{1}{\sum_{i=1}^N w_i^2}. \quad (6)$$

We adopted the sampling importance resampling (SIR) algorithm, in which particles with the weight w_i

of less than $1/N$ are replaced by particles stochastically drawn from all samples at the resampling step. Moreover, the adaptive $\mathbf{R}$ estimator (ARE) based on the Bayesian estimation proposed by Ueno and Nakamura (2016) is incorporated into the particle filter with the JMANHM. Because the weight w_i is a function of $\mathbf{R}$, the optimal $\mathbf{R}$ matrix at each resampling step is expected to produce reasonable weights, and consequently, is expected to avoid filter degeneracy. Hereafter, we refer to the particle filter with JMANHM and ARE as NHM-RPF.

Considering the effectiveness of ARE, we implemented advanced observational operators originally developed for NHM-4DVAR of conventional observations, Doppler radial velocity data by weather radars, Global Navigation Satellite Systems (GNSS)-derived integrated water vapor (Kawabata et al. 2007), zenith total delay, slant path delay data (Kawabata et al. 2013), radar reflectivity data (Kawabata et al. 2011), Doppler wind lidar data (Kawabata et al. 2014), and dual polarimetric radar data (Kawabata et al. 2018a; Kawabata et al. 2018b).

Because computational cost is an important issue for particle filters with high-dimensional weather prediction models, and the file input–output (IO) time in particular accounts for the greatest cost, we designed the ensemble system for NHM-RPF to use the message passing interface (MPI) technique, different from the usual script-based ensemble systems. The MPI ensemble system first run in the single MPI world and then is paralleled. Therefore, the resampling step is performed by MPI communication without performing any file IO procedures. In addition, we decided to continuously perform time integration (without stopping the computation job) through the DA period with the filtering step at observation times, whereas the typical DA procedure and time-integration step are performed one after the other (the DA–forecast cycle). In typical systems, a new cycle begins when new lateral boundary conditions are provided by the outer models in a nested system; however, this procedure is not necessary in our OSSE, which uses a short DA period of 90 min and a hindcast setting.

3. Observing system simulation experiment

a. Settings and methodology

We conducted an OSSE to investigate PDFs during the CI and development stages. During this experiment, referred to hereafter as “PF,” we used 1000 ensemble members to perform 90 min of sequential DA. The DA is performed every 10 min for $48 \times 48 \times 50$ grids with a horizontal grid spacing of 2 km. Note that, for simplicity, we used only conventional observational operators.

FIG. 1. Experimental domains for the (a) LETKF at 15-km grid spacing, (b) LETKF at 2-km grid spacing, and (c) OSSE at 2-km grid spacing with 48×48 grids. The topographic contour interval is 500 m. (d) Experimental time-setting. Black circles denote two time steps for the lagged ensemble method.

For comparison, we conducted an ensemble simulation experiment with the same settings but without any DA (a free-running ensemble), referred to hereafter as “NoDA.”

To create the initial and boundary conditions for the OSSE, a local ensemble transform Kalman filter (LETKF; Hunt et al. 2004) for JMANHM (Kunii 2014) was used. Its run was conducted over the Japanese Islands (Fig. 1a) with a horizontal grid spacing of 15 km from 0000 UTC 1 August to 0000 UTC 3 August 2016. The DA was performed every 6 h by assimilating conventional data. The aim was to produce lateral boundary conditions for a higher-resolution LETKF system with a smaller domain at the 2-km grid spacing (Fig. 1b; $122 \times 122 \times 50$ grids), which was run from 1200 UTC 2 August to 0000 UTC 3 August. During this run, conventional, GNSS integrated water vapor (Shoji 2013) and radial velocity observations were assimilated every 3 h. The experimental domain of the OSSE (Fig. 1c) was part of the high-resolution LETKF domain and the DA period was from 2100 to 2230 UTC 2 August. This time setting is summarized in Fig. 1d. Saito et al. (2019) investigated perturbations in a cloud resolving the LETKF system in the same case.

A nature run (Fig. 2) used in the OSSE was a member of the 51-member ensemble (50 members plus the ensemble mean) that started at 2100 UTC 2 August. Pseudo-surface observations of potential temperature (K ; hereafter PT); wind (m s^{-1} ; hereafter U and V); water vapor mixing

ratio (g kg^{-1} ; hereafter QV) at 20 m (blue circles in Fig. 2); and pseudoradar observations of the rainwater mixing ratio (g kg^{-1} ; hereafter QR) at 0.84, 1.94, 3.49, and 5.49 km (red circles in Fig. 2), covering the initiation and development area of the cumulonimbus in the nature run, were assimilated. In terms of the observational error matrix, we considered $\mathbf{R}$ as diagonal in the present study, and the Gaussian random errors of 2.0 K, 1.0 m s^{-1} , 10.0, and 10.0 g kg^{-1} were added to the PT, U , V , QV, and QR observations, respectively. The total number of observations was 48 and they were assimilated every 10 min.

To create 1000 initial and boundary conditions, first, the lagged ensemble method was applied with the high-resolution LETKF at 1800 UTC, in addition to the ensemble initiated at 2100 UTC, to obtain a 100-member ensemble. The ensemble size was then increased to 1000 by generating 900 members from Gaussian random variables with mean and covariance matching the ensemble mean and ensemble covariance, respectively, of the 100 members. These new members were expected to maintain the dynamical and thermodynamical structures of the original ensemble. Therefore, they were less noisy in comparison to ensembles generated using white noise. This procedure means that the initial PDFs were discretized first to the 100 members and then to 1000 members.

The same procedure described in the aforementioned paragraph was applied to the lateral boundary conditions. These various lateral boundary conditions

FIG. 2. Nature run. Horizontal distributions of the mixing ratio of QR (color scale) and horizontal winds U and V (arrows) at 3.49-km height at (a) 40, (b) 60, and (c) 90 min after the initial time. Vertical cross sections of the mixing ratio of total liquid (rain, snow, graupel, and hail; color scale), and three-dimensional winds projected onto the plane of the cross section (arrows) along gray line A–B in (c) at (d) 40, (e) 60, and (f) 90 min. Blue circles in (a)–(c) represent the locations of U , V , PT , and QV observations at the lowest level of 20 m above the ground level, and red circles represent QR observation points at heights of 0.84, 1.94, 3.49, and 5.49 km.

were considered to be system noise included in the temporal evolution model of x . This was expected to maintain a large ensemble spread during the experiment.

In this study, we used the root-mean-square error (RMSE) and spread to verify and discuss the results. The RMSE was calculated as follows:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{j=1}^n (a - \bar{x})^2}, \quad (7)$$

where n is the number of grids and a and $\bar{x}$ are the prognostic variables of the nature run and the ensemble mean of x , respectively. The spread was calculated as the standard deviation of the ensemble as follows:

$$\text{spread} = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2}. \quad (8)$$

To evaluate RMSEs in total over the experimental period, the improvement rate (%) is defined as follows:

$$\text{Rate}_{\text{improve}} = \frac{1}{N_{\text{it}}} \sum_{\text{it}=\text{itst}}^{\text{itend}} \frac{\text{RMSE}_{\text{ref}} - \text{RMSE}_{\text{test}}}{\text{RMSE}_{\text{ref}}} \times 100, \quad (9)$$

where N_{it} is the number of DA (nine in this case), itst and itend are the beginning and end of the DA (10 and 90 min, respectively, in this case), RMSE_{ref} is the RMSE of a reference case (NoDA in this case), and $\text{RMSE}_{\text{test}}$ is the RMSE of a test case (PF in this case). A positive rate value indicates improvement while a negative value indicates degradation.

Finally, the Bayesian Information Criterion (BIC; Akaike 1977; Schwarz 1978) was introduced to evaluate the Gaussianity of the PDFs (Ueno and Tsuchiya 2009) as follows:

$$\text{BIC} = -2 \ln \ell + m \log N, \quad (10)$$

where ℓ is the likelihood of data assumed to follow a given statistical model and m is the number of parameters of the statistical model. We used BIC to examine three statistical models: a unimodal Gaussian model, a

FIG. 3. Time series of the ESS (bold black) by Eq. (6) and the maximum weight (thin blue) at each resampling step.

bimodal model comprising a two-Gaussian mixture (McLachlan and Peel 2000), and a histogram model (Sakamoto et al. 1986). The histogram model is a multinomial distribution model that has parameters representing the number of classes. A smaller BIC value indicates a better model.

Note that all figures from the PF (histograms, ensemble means, RMSEs, spreads) presented in the following sections were created with priors.

b. Nature run

In the nature run, winds were southerly and a convective rain area formed (convection initiation: CI) in the central area of the domain at 40 min after the initial time (Fig. 2a). Updrafts were seen underneath the cloud (Fig. 2d) and the cloud elongated northward; eventually, it developed a horizontal extent of approximately 10 km at 60 min (Fig. 2b). The updrafts in the convection core strengthened and the convective cloud grew vertically (Fig. 2e). By 90 min, the cloud had developed into a cumulonimbus as its top had reached a height greater than 10 km (Fig. 2f). Because of the southerly winds, the cumulonimbus moved northward during its lifetime. In summary, the nature run well simulated the initiation and development of a cumulonimbus.

c. Results

Filter collapse is a matter of concern for particle filters, which depend on the degree of freedom measured by observations and their accuracy; therefore, we carefully designed the observational network to avoid filter collapse while still capturing the cumulonimbus in the nature run.

FIG. 4. Time series of RMSEs (black lines) and spreads (gray lines) of PF (solid) and NoDA (dashed) for (a) PT, (b) QV, (c) QR, (d) U, (e) V, and (f) W over the entire assimilation domain against the nature run at assimilation times from 10 to 90 min.

(a) PF

(b) NoDA

FIG. 5. As in Figs. 2a–c, but for (a) PF, and (b) NoDA. The red box in (a) at 40 min is the display domain for Figs. 7, 9, and 10. The purple line S–N in (a) is the vertical cross section shown in Fig. 6.

The ESS at each assimilation step, given by Eq. (6), and the maximum weight at each resampling step are shown in Fig. 3. The ESS remained larger than 100 until 80 min, although one at 90 min dropped to 40. This stability was because of the system error from the various lateral boundary conditions described in section 3a and the ARE, whose effect is examined in detail in section 4c. In addition, because the maximum weight among all 1000 particles was only 5.9% even at 90 min, we can conclude that NHM-RPF had successfully avoided filter collapse during the OSSE.

Next, we compared the three-dimensional fields (grid-to-grid) of the nature run to those of PF and NoDA (Fig. 4). The RMSEs of PT, QV, QR, and three-dimensional wind fields in PF (solid black line) were clearly less than those in NoDA (dashed black line). Even though the differences in the RMSEs of QR and

W were relatively small, the other RMSEs showed significant improvement. In addition, we calculated spreads (gray lines in Fig. 4). Similar to the RMSEs, spreads in PF were smaller than those in NoDA over the DA period.

The QR ensemble means show that at 40 min, CI was not captured in NoDA (Fig. 5b), while it was in PF (Fig. 5a). In NoDA, although the cumulonimbus developed from 60 to 90 min, the QR intensities at 60 min were much weaker than those in the nature run (Fig. 2) whereas the QR intensities were substantially improved in PF and comparable to the nature run at 90 min. Note that the intensities shown in Fig. 5 are ensemble means; therefore, they were inevitably weaker than those in the single simulation of the nature run. In PF, the cloud top reached a height greater than 10 km, as in the nature run, but did not in NoDA (not shown).

FIG. 6. Vertical cross sections along the purple line in Fig. 5a of $dLCL$ (shaded), winds (arrows), and the mixing ratio of rainwater (green contours) at (a) 10 and (b) 40 min. Cross mark represents the grid D in Fig. 7e. The x axis represents the distance (km) from the south border of the experimental domain.

The results of these verifications clearly show that the ensemble means of PF were much closer to the nature run than those of NoDA. Moreover, because the PDFs of PF were more closely distributed around the nature run than those of NoDA, the spreads were reduced, maintaining a proper size. Therefore, we concluded that NHM-RPF successfully reduced the NoDA errors by assimilating observations through the particle filter process. Furthermore, only PF well represents the convection intensity and the timing of CI.

4. Discussion

a. Mechanisms of convection initiation

To understand the mechanism of CI, we examined vertical cross sections along the inflow wind direction of $dLCL$ (difference in lifting condensation levels), winds, and QR at 10 and 40 min (Fig. 6). $dLCL$ is defined as the height difference between the condensation level of an air parcel and the height at which the parcel is originally lifted from. Small $dLCL$ values indicate static instability at the height of the parcel. The cross section passed across the grid D in Fig. 7e (cross mark in Fig. 6). In addition, the PF ensemble means of PT, QV, relative humidity (RH), cloud water mixing ratio (QC), QR, and vertical wind (W) from 10 to 60 min over the CI region are shown in Fig. 7.

Figure 6 shows two air masses: one with a high $dLCL$ greater than 300 m in the upper-south region and the other with a low $dLCL$ less than 100 m in the lower-north region. The former was stable, warm, and dry whereas the latter was unstable and wet (see Fig. 7). It is clear that the grid D (cross mark) is in the frontal boundary area between these two at 10 min. Moreover, updrafts were observed in the area underneath grid D, which is the wet and unstable air (Fig. 6a). These updrafts led to

cloud initiation in the upper boundary of the air with strong updrafts at 40 min (Fig. 6b).

From Fig. 7, at 10 min, it is also clear that the warm, dry air mass was intruding into this region from the south. Updrafts and high RH ($>90\%$) in the frontal boundary of the air mass led to the generation of a cloud at 20 min (Fig. 7d) and the associated saturation and condensation processes warmed the surrounding air. At 40 min, RH exceeded 95% and QV was greater than 10 g kg^{-1} ; this humid air converted to cloud water at greater than 1.0 g kg^{-1} and further to rainwater at greater than 1.0 g kg^{-1} with an updraft of 1.4 m s^{-1} . This CI process appears to be typical cloud initiation. As the cloud developed, it moved northward, similar to the nature run. In summary, lifting ahead of a frontal boundary within an unstable environment caused CI.

b. PDFs of convection initiation and development

We investigated PDFs at selected grid points (see Fig. 7e) during this process (Fig. 8). These points were chosen to include the CI point, the region of inflow into the CI, and the development region. Note that the PDFs discussed in this subsection are for prior errors.

At 10 min, the PDFs of PT, QV, RH, and W appeared to be mostly Gaussian whereas those of QC and QR were concentrated in the no-water region of the leftmost bin. Note that the PDF of W in grid D showed a markedly skewed distribution because of the strong updrafts in some members of the ensemble. At 20 min in the same grid D, the PDF of RH became non-Gaussian in shape, and that of QV was also relatively flattened and non-Gaussian. Also, at 20 min, weak QC probabilities were observed in the water-rich region in the same grid D and the ensemble mean of QC exceeded 0.1 g kg^{-1} (Fig. 7d). As described in the previous subsection, the ensemble means showed the convective cloud was initiated by the

FIG. 7. Ensemble means of (a) PT, (b) QV, (c) RH, (d) QC, and (e) QR at 2.82-km height in PF within the red box in Fig. 5a. Contours show updrafts at 1.23-km height (contour interval 0.2 m s^{-1}). The red cross marks in (e) at 10 min show the sampling grid points for Fig. 8.

updraft. It is obvious that this was related to the skewed PDF of W at 10 min.

At 30 min, as the cloud developed, the PDFs of W in the more northerly area (grids A–D) became non-Gaussian and quite skewed. At the same time, the PDFs of RH in these grids showed clear non-Gaussian distributions and, owing to the upper bound of RH

(up to 100%), the PDFs of RH and QV also showed bimodal distributions.

The ensemble mean of QR reached greater than 0.5 g kg^{-1} at 40 min (Fig. 7e) and, at the same time, QR probabilities greater than 1 g kg^{-1} (the midpoint of the x axis) appeared in grid C. The PDF of QC also became markedly bimodal, with two widely separated peaks in the no-water and 1 g kg^{-1} regions of the x axis. The higher peak was also at the upper bound of QC, because in the numerical model, cloud water is automatically converted to rainwater as part of the cloud microphysical process when its mixing ratio exceeds a certain value. At 40 min, all the PDFs at grid D were quite non-Gaussian in shape. Therefore, the PDFs during the CI indicated quite non-Gaussian processes. Moreover, it is implied that the non-Gaussian PDFs in RH originated with that in W and its upper bound of 100%. The non-Gaussianity of RH and W created that of PT and QV. These non-Gaussian PDFs were maintained as the convection developed and moved northward from 50 to 60 min.

We calculated the BIC for only PT, QV, RH, and W because it did not make sense to evaluate the Gaussianity of the completely non-Gaussian PDFs of QC and QR. We evaluated the non-Gaussianity of PT, QV, RH, and W by showing the superiority of a Gaussian mixture or histogram model to the Gaussian model, as indicated by their BIC values (Fig. 9). In addition, ensemble spreads of these variables are also shown in Fig. 10.

Similar to Fig. 8, the PDFs of W (Fig. 9d) showed non-Gaussianity even before the CI, the Gaussian mixture was selected as the best model in the area where the convective cloud initiated, and the spreads were also large in this area. In addition, unlike the large spreads, the non-Gaussianity of W dominated the entire domain and remained even after the convective cloud had passed. Similarly, the PDFs of RH were dominantly non-Gaussian, although around the CI area, the best model for the non-Gaussianity of RH was the histogram. In contrast, the PDFs of PT and QV (Figs. 9a and 10b) were initially Gaussian; however, after 30 min, non-Gaussian PDFs dominated the entire domain. The non-Gaussian PDFs of PT were associated with the CI and development; however, once the convective cloud had moved away, they recovered their Gaussianity (see the southern area of the domain at 60 min).

In contrast, the spreads of PT, QV, and W showed similar horizontal distributions to each other (Fig. 10) and the larger spreads were distributed near the peaks of the ensemble means of W , RH, and QC (Fig. 7) and also near the horizontal distributions of non-Gaussianity in RH. These results indicated that particles diversified where convection occurred, although these variables

FIG. 8. Probability densities of PT, QV, RH, W, QC, and QR at grid points of A, B, C, D, and E (shown in Fig. 7e). The maximum frequency shown on the y axes is 50%, and the x axes are each divided with 20 bins. For PT, QV, and W, the x axis shows gridpoint values between the minimum on the left and the maximum on the right; for RH, values on the x axis range from 50%–100%, and for QC and QR, values on the x axis range from 0.01 to 1.0 g kg⁻¹ and from 0.1 to 10.0 g kg⁻¹, respectively, in log scale. Note that the medians of PT, QV, and W are fixed at the middle of the x axis, because their maximum and minimum values are individually determined at every grid and time, whereas the medians of RH, QC, and QR are not fixed.

FIG. 9. The distributions of the selected statistical models for (a) PT, (b) QV, (c) RH, and (d) W at 2.82-km height in the same domain as in Fig. 7. Gray, blue, and red represent Gaussian, Gaussian mixture, and histogram models, respectively.

were strongly related to each other through thermodynamic and cloud microphysical laws.

The difference between the PDFs of PT, which recovered their Gaussianity at 60 min, and those of QV, which remained non-Gaussian, is interesting. The difference between these two variables was possibly a result of QV not being a conservative variable; thus, it was difficult for QV with a Gaussian PDF to be advected from the outer domain.

For an examination of the non-Gaussianity initiation process, vertical cross sections of the spreads of RH and W , a correlation map of QV and W , and selected statistical models for W at 10 min are shown in Fig. 11. Although the air in the low-north region was wet (Figs. 6a

FIG. 10. As in Fig. 9, but for spreads.

and 7), the spread of RH was less than 2% (Fig. 11a) while the spread of W was relatively large: the spread was 0.14 ms^{-1} at the grid D and the average was 0.02 ms^{-1} . In contrast to the average, the median was -0.01 ms^{-1} and the average of the top 100 members was 0.33 ms^{-1} . Thus, the updrafts of only a small number of members were strong. This variability may originate from the intensity and/or timing of the frontal boundary. The cross correlations between W at grid D and QV show that high correlations existed in the upper boundary area. Self-correlations against W at grid D illustrate that the updrafts were highly correlated vertically, even above the upper boundary. These correlations show that the updrafts transported the abundant water vapor existing in the wet air mass from the lower troposphere (lower than 2000 m) to the mid-troposphere (higher than 3000 m). This led to the initiation of the cloud at 3000 m in height at 30 min and then rainwater at 40 min. Therefore, the large variability in W was connected to that of the cloud initiation and the

(a) Spreads of RH and W

(b) Correlation map of QV and W

(c) Selected statistical models for W

FIG. 11. As in Fig. 6, but for (a) spread of RH (shaded) and W (contours), (b) cross correlations of QV against W (shaded) and self-correlation of W (contours) at the grid D, and (c) the selected statistical models for W. The present time is 10 min.

non-Gaussianity of the cloud meteorological conditions. The variability (large spread) was evaluated as non-Gaussian by BIC (Fig. 11c) and the non-Gaussianity of W was distributed in the lower troposphere and even above it over grid D.

From these results, we can conclude that the PDFs became strongly non-Gaussian when NHM-RPF produced diverse particles during the CI and development period. This transformation was led by the non-Gaussian PDF of W at the beginning and then the upper-bounded PDF of RH produced the non-Gaussian PDFs of QV and PT. The non-Gaussianity of the PDFs of QC and QR was quite high throughout the experimental period. Some PDFs of QC and QR remained in the no-water region after the cloud had developed into a cumulonimbus; thus, even during the developmental stage, their distributions were bimodal, with widely separated peaks, one of which was always in the leftmost bin. This is an interesting feature that was not seen in the other variables.

c. Effect of adaptive $\mathbf{R}$ estimation (ARE)

We examined the effect of the ARE by applying a fixed $\mathbf{R}$ in the PF experimental setting. This test case,

hereafter referred as PF_woARE, was the same as that of PF but ARE was not applied. In PF_woARE, the observation errors were not changed from the initial values throughout the entire experimental period, which were also given as the initial values for PF.

First, we show the ESS and maximum weights in PF_woARE (Fig. 12). In comparison to Fig. 3, although the maximum ESS number is similar, the maximum weights and ESSs were strongly uncorrelated from 10 to 60 min. Moreover, ESSs after 50 min in PF_woARE are less than 60. This illustrates that PF_woARE is not stable and near filter collapse. Table 1 shows the improvement rates for PT, QV, QR, U , V , and W in PF and PF_woARE compared to NoDA. The values of PF are all positive and between 14% and 25% while those of PF_woARE are negative between -29% and -61% . This result demonstrates that PF had clearly improved accuracy compared to that of NoDA, while PF_woARE did not. Thus, we can conclude that the ARE provides stable filtering in the particle filter as well as an improvement in accuracy.

Next, estimated observation errors were examined (Fig. 13). Because the error variances mostly varied less

FIG. 12. As in Fig. 3, but for additional experiments of PF_woARE.

than five times the initial values, it can be said that the estimated $\mathbf{R}$ had a realistic range. However, several changes of greater than 20 times are seen in U and V . Particularly, three U observation values were greater than 50 times the initial value (in red). We found that these were likely related to the large difference between the observations and ensemble mean values. For instance, the U observations at 70 and 90 min colored in red (Fig. 13a) are apart from the ensemble means by -9.4 and 5.1 m s^{-1} whereas nearly all the other absolute differences were less than 1.0 m s^{-1} . One of the reasons for this was that when we produced the pseudo-observations, we added Gaussian errors to the truth. This process has the potential to stochastically add quite large errors; this actually happened in our observations. It was found that two observations were given a large difference from the truth. For instance, the error of 9.8 m s^{-1} was given to a truth of -0.01 m s^{-1} and a U observation of 9.79 m s^{-1} was created, even though the default error for wind observations was 1.0 m s^{-1} . However, these large estimated errors are evidence that the ARE estimated true observational errors appropriately.

Other relatively large error changes were likely connected to the large variances in innovations (Fig. 13b). For instance, it is recognized that large error changes in QR (the upper half of Fig. 13a) exist along the large variances (upper half of Fig. 13b), which are related to cloud development and movement.

In summary, because the error changes and innovation variances in PT and QV are relatively small, it can be said that these represent a larger scale than the cloud initiation and development scale. Large changes and variances in QR are directly connected to cloud initiation and development and these in U and V are affected by relatively large observational errors.

d. Impact of the number of observations

To investigate the impact of the number of observations, we installed new observational networks over

TABLE 1. Improvement rates (%) of RMSEs against NoDA.

	PT	QV	QR	U	V	W
PF	21	24	14	17	25	18
PF_woARE	-29	-39	-55	-42	-49	-61

the experimental domain (Fig. 14) that were designed considering a linear increase in observation density. SfcXX represents the horizontal observations points and RadXX illustrates the vertical locations of QR observations. We examined all combinations of SfcXX and RadXX. For instance, the experiment Sfc17Rad04 used 17 observation points for surface observations at the lowest level, and radar observations at four vertical levels, totaling 136 observations $[(U, V, PT, QV) \times 17 + QR \times 17 \times 4 = 136]$. The detailed observational networks are explained in the caption of Fig. 14. The total number of experiments described in this subsection was 25.

The RMSE improvement rates are shown for all observational network experiments (Table 2). The bold numbers represent a greater improvement. An increase in the horizontal observation density (y axis) shows mostly linear improvement of RMSEs for all elements. Meanwhile, the increase in vertical levels (x axis) is not sensitive. This is caused by the different number of observations in the horizontal and vertical planes and the relatively large observation error in QR. The improvement rates in U and V are similar to those of the other elements (not shown).

From the ESS of each experiment, we found that the ESSs of Sfc25 and Sfc37 were less than 3.0 (Table 3) even when they used Rad01 in the vertical directions. Thus, it can be said that these experiments mostly collapsed. From the improvement rates of the RMSEs, it seems that the RPF provides improvements for any increase in observations and this increase benefits accuracy (Table 2). However, in fact, a large number of observations limits the particle filtering stability even with the RPF. In the case that the number of observations is large, it is likely that only a few particles fit to the observations; thus, the NHM-RPF distributes the particles around the observations in a narrow PDF space. This hardly occurs in a real case, because, unlike the OSSE in this study, real observations should exist outside of the PDFs spanned by a small number of particles.

5. Summary and conclusions

A particle filter based on a sampling importance resampling algorithm with the JMA nonhydrostatic model and an adaptive $\mathbf{R}$ estimator (NHM-RPF) was

FIG. 13. Time series of (a) estimated observation error variances and (b) variances of innovations. Each observation is shown on the y axis and DA time is on the x axis. The numbers on y axis (1–6 and 1'–6') represent observation points and L and H in the QR observations illustrate vertical levels (lower and upper). The errors and variances are normalized by the initial values. Note that only the innovation variances of QR are shown in log scale.

FIG. 14. Observation networks. (left) The white large box represents the whole experimental domain (see Fig. 1c). Colored boxes are observation points, and different colors illustrate different set of observation network for (top right) the Sfc04–37 experiments. Radar observations (QR) locate above the colored boxes at height levels of 0.53, 1.45, 2.82, 4.64, and 6.91 km. The Rad01–05 experiments used from 1 to 5 levels, which were incrementally increased from lower to upper levels.

developed. The aim was to investigate non-Gaussianity in probability densities of parameters during convection initiation and development in connection with their mechanisms. Unlike typical script-based ensemble systems, NHM-RPF was parallelized in the ensemble space using the MPI technique to reduce the file input–output time, which constituted a large part of the total computational cost. In addition, advanced remote sensing observational operators were implemented.

An OSSE was conducted with NHM-RPF. In the OSSE, a short assimilation period (90 min), small domain ($48 \times 48 \times 50$ grids), 2-km storm-scale grid spacing, relatively small number of observations (48), and a large number of particles (1000) were used. This setting was

carefully designed to avoid the “curse of dimensionality” in particle filters. For instance, Snyder et al. (2008) showed that it is necessary for particle filters to exponentially increase the number of ensembles by the dimension of problems.

For a nature run, a simulation of a well-developed cumulonimbus from the ensemble simulation was chosen. Pseudo-observations of horizontal wind, potential temperature (PT), and water vapor mixing ratio (QV) data at the surface level, and rainwater mixing ratio (QR) data in the lower troposphere, were created and assimilated every 10 min.

Because the effective sample sizes throughout the entire assimilation period were sufficiently large and the

TABLE 2. Improvement rates of RMSEs against NoDA. Boldface numbers represent improvement rates greater than or equal to 20%.

PT						QV					
	Rad01	Rad02	Rad03	Rad04	Rad05		Rad01	Rad02	Rad03	Rad04	Rad05
Sfc04	5	12	9	9	3	Sfc04	5	12	8	11	–2
Sfc09	11	13	15	11	8	Sfc09	9	14	18	19	2
Sfc17	28	28	21	25	25	Sfc17	30	31	26	28	27
Sfc25	33	32	31	29	34	Sfc25	36	37	36	37	39
Sfc37	33	35	33	31	34	Sfc37	37	41	38	39	40
W						QR					
	Rad01	Rad02	Rad03	Rad04	Rad05		Rad01	Rad02	Rad03	Rad04	Rad05
Sfc04	5	12	8	9	2	Sfc04	3	11	7	8	2
Sfc09	6	9	12	13	6	Sfc09	5	8	12	12	6
Sfc17	19	20	13	19	19	Sfc17	16	17	11	16	17
Sfc25	22	23	22	23	25	Sfc25	21	21	19	20	22
Sfc37	24	24	24	20	24	Sfc37	20	20	21	18	21

TABLE 3. ESS with the first value less than or equal to 3.0 and its time step (min). Cross marks represent experiments which never had an ESS value less than 3.0.

	Rad01	Rad02	Rad03	Rad04	Rad05
Sfc04	×	×	×	×	×
Sfc09	×	×	×	×	2.5 (50)
Sfc17	×	×	2.6 (70)	×	×
Sfc25	2.6 (10)	2.6 (70)	×	3.0 (70)	2.6 (10)
Sfc37	1.9 (10)	1.9 (10)	1.9 (10)	1.9 (10)	2.1 (10)

maximum weight was less than 6%, it was shown that the filtering results (the PF case) did not undergo filter collapse. Moreover, the PF was verified by calculating the RMSEs against the nature run. The results illustrated that PF showed a significant improvement against a free-running ensemble simulation without any data assimilation (NoDA). In addition, spreads in PF were smaller than those in NoDA. The ensemble mean of rainwater in PF was similar in intensity and distribution to that in the nature run but not that in NoDA.

In the ensemble means of PF, the convective cloud initiated by lifting ahead of a frontal boundary within an unstable environment, which caused CI and the cloud moved northward as it developed (Fig. 7).

The examination of the PDF histograms during the PF experiment (Fig. 8) showed that at 10 min, the probability distributions of RH and W at the site of CI were non-Gaussian in shape and that those of QC and QR were restricted to the no-rain region whereas the PDFs of PT and QV appeared to be Gaussian before CI. Because RH had an upper bound of 100%, water vapor saturation and condensation played an important role in the generation of non-Gaussianity during CI. As the convective cloud developed, the probabilities of QC and QR shifted to water-rich regions and the PDFs of PT and QV became non-Gaussian.

To evaluate non-Gaussianity, we applied the Bayesian information criterion (BIC). BIC was used to select the best-fitting statistical model, between Gaussian, two-Gaussian mixture, or histogram models, to the ensemble results (Fig. 9). Furthermore, we examined the ensemble spreads (Fig. 10). The model selection and spread results showed that the PDFs of W were the first to become non-Gaussian during CI followed by those of RH; they remained non-Gaussian even after the convective cloud moved away. Before CI, the PDFs of QV were Gaussian, but afterward they became non-Gaussian. The PDFs of PT were non-Gaussian during CI but quickly recovered to Gaussian after the convective cloud moved away. As a next step in our studies, we will investigate why the PDFs of some variables recovered Gaussianity while others did not. It will also be interesting to investigate what causes the difference in selected

models in non-Gaussian areas, a two-Gaussian, and a histogram model. In addition, another issue is an investigation of the origin of these non-Gaussian shapes. It will be interesting to explore how these shapes form.

During CI and development, a non-Gaussian PDF of W was first generated by particles with a strong updraft. This was connected to variabilities in saturation and condensation processes as the next source of non-Gaussianity. Autoconversion in the model process led to bimodal PDFs of water substances.

In addition, we examined the effects of the adaptive $\mathbf{R}$ estimator (ARE) and the number of observations. The ARE resulted in a significantly improved accuracy in PF and stable filtering in the case in which the number of observations increased. In these impact tests, the estimation of $\mathbf{R}$ played an essential role. From Eqs. (2) and (5), a large $\mathbf{R}$ assigns nearly equivalent weights to every particle thus lacking filtering effects. In contrast, a small $\mathbf{R}$ imposes weight to a single particle, which leads to filter degeneracy. Maximizing the posterior on $\mathbf{R}$ maximizes the mean of the likelihoods of all ensemble members subject to the prior constraint. With a reasonable $\mathbf{R}$, we can conduct filtering based on observations and avoid filter collapse. For stable particle filters, a localized particle filter (Poterjoy 2016; Potthast et al. 2019) would be an alternative.

We clarified the propagation of non-Gaussianity during CI and development, but some challenges remain. Because the OSSE started with an ensemble initiated with LETKF, the PDFs at the beginning of the experiment were Gaussian in shape. In the future, we will conduct simulations over much longer time periods in a larger domain that includes several CI events. This will make the settings used in the present study more realistic.

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