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Estimation of ecotype-specific cultivar parameters in a wheat phenology model and uncertainty analysis

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ABSTRACT

The objective of this study was to develop an effective method for predicting ecotype-specific cultivar parameters for the large-scale application of wheat crop simulation models. The Markov Chain Monte Carlo (MCMC) technique was explored for parameter calibration based on an existing model. We estimated the posterior probability distribution of ecotype-specific cultivar parameters at four ecosites (Huai'an, Zhengzhou, Weifang, and Shijiazhuang in China) by using the historical phenological stages of wheat and daily weather data from 1980 to 1995. 1000 sets of cultivar parameters which were randomly sampled from the posterior probability distribution at each ecosite from 1996 to 2005 were used to evaluate the MCMC-based method. Optimal 50 sets of parameters were chosen from the 1000 sets of parameters at each ecosite to represent the ecotype-specific cultivar parameters of the Jiangsu, Henan, Shandong and Hebei provinces to evaluate the MCMC-based method for the year 2005 at the regional scale. The results showed that the coefficients of determination (R^2) between the observed and estimated phenological stages ranged from 0.61 to 0.72, with a root mean square error (RMSE) of less than 3.6 days and a root mean square deviation $\left(\overline{\mathrm{RMSD}}\right)$ of less than 3.7 days at the site scale. All of the RMSE and $\overline{\mathrm{RMSD}}$ values for the three phenological stages obtained using the posterior probability distribution at the four ecosites were significantly lower than those based on the prior probability distribution. At the regional scale, R^2 between the observed and estimated phenological stages was greater than 0.86, with RMSE less than 3.4 days and $\overline{\mathrm{RMSD}}$ less than 4.0 days in most of the grids for year 2005. The estimated phenological stages agreed well with the observations, suggesting that the MCMC technique has high reliability of for estimating multiple parameter combinations in a wheat phenology model. The combination of the present MCMC technique and a phenology model could be used for estimating the ecotype-specific cultivar parameters for the main wheat growing regions of China, which can be used to predict progress of wheat development at the regional scale.

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1. Introduction

Crop simulation models have been widely used to predict grain productivity, precision crop management, regional agricultural design, and are considered as an important method for quantitative evaluation of agricultural production systems (Liu et al., 2002). Many of these simulation analyses are based on site-specific predictions. At the regional scale, however, significant spatial variations exist in agricultural production environments (climate conditions and soil characteristics) and management systems (Priya and Shibasaki, 2001; Shi et al., 2009). In turn, accurately applying a crop simulation model at the regional scale remains a challenging problem in the field of agricultural system analysis.

In recent years, studies have been carried out on the regional application of crop models. Priya and Shibasaki (2001) integrated environmental policy integrated climate (EPIC) model with a geographic information system (GIS) and established a spatial crop yield estimating system (Spatial EPIC). Shi et al. (2009) constructed a system for predicting and evaluating regional wheat productivity based on a wheat simulation model (WheatGrow) and GIS. In general, these models require input of various regional parameters, including regional cultivar parameters, management practices, as well as weather and soil data. Yet determination of cultivar parame-

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ters at the regional scale is a complex process, limiting the effective application of crop simulation models to regional scale predictions (Iizumi et al., 2009).

When a crop simulation model is extended from a site to a regional scale, the performance of a specific cultivar becomes less important. Instead, an integration of the main cultivars in the region is considered representative of an ecotype cultivar needed for predicting the regional productivity (Iizumi et al., 2009; Shi et al., 2009; Tao et al., 2009). The climatic ecotype is one type of ecotype. This climatic ecotype cultivar should have common characteristics of main cultivars grown in the region, such as regional climate adaptation after long-term crop selection. Therefore, the climate ecotype-specific cultivar parameters are related to regional climate and are considered constant within an ecological zone. For example, the parameters that determine the phenological characteristics have shown no clear scale dependency or, at most, weak scale dependency (Iizumi et al., 2014). Other parameters are cultivar-specific and differ across cultivars within an ecological zone. Parameters related to phenology are considered climate ecotype-specific cultivar parameters and are used for regional simulation in a wider region.

Yet it is difficult to obtain ecotype-specific parameters with traditional field-testing procedures (He, 2008). Thus, an estimation method is needed for generating ecotype-specific parameters using regional historical data of weather conditions, crop phenology, and yield. Jin and Shi (2006) adopted a trial and error method to determine the ecotype-specific parameters using the time series yield data and weather conditions at a county scale. Xiong et al. (2007) also applied the trial and error method to calibrate ecotype-specific parameters for simulating regional maize production with the CERES-Maize model. Several other methods are used for estimating these parameters, such as genetic algorithms (Dai et al., 2009) and simulated annealing method (Ferreyra, 2004). However, these methods present a partially optimal rather than globally optimal combination of model parameters and do not reflect the characteristics of similar impacts of different parameters (i.e., different combinations of the parameters tend to produce similar simulation results) (He et al., 2009). To solve this problem, some researchers have used the Bayesian approach to obtain a posterior distribution of a parameter based on a prior distribution and an observed dataset for optimizing the parameters of a multivariate nonlinear model. This approach is becoming popular in regional simulation studies and has been used with a crop growth model (Iizumi et al., 2013), a canopy transpiration model (Samanta et al., 2007) and a terrestrial ecosystem model (Harmon and Challenor, 1997; Xu et al., 2006). Other researchers have confirmed the benefits of using this methodology for impact assessment in the fields of forest, biogeochemistry and groundwater flow (Van Oijen et al., 2005; Arhonditsis et al., 2008; Hassan et al., 2009).

The Bayes' approach (Gill 2002; Braswell et al., 2005; Raupach et al., 2005; Van Oijen et al., 2013) requires two types of information: prior information based on expert knowledge and data collected via experimentation. Its basic principle is to start with a prior probability distribution of crop model parameters, which describes our perception of the parameter values before experimental observations. Through updating prior parameter distributions and using the measurements, the Bayesian framework produces posterior parameter distributions (Makowski et al., 2006). Due to the complexity of crop models (non-linearity, high number of parameters), it is almost impossible to analytically calculate the posterior parameter distributions (Gelman et al., 2004). However, the growing power of computers and the development of new methods make the Bayesian approach more accessible even for complex models (Makowski et al., 2002). The Markov Chain Monte Carlo (MCMC) methods are effective in solving this problem (Hassan et al., 2009). The method is based on the Bayesian theoretical framework to establish a balanced distribution of the Markov chain and samples from its balanced distribution. By continuously updating the sample information, the chain fully searches parameter intervals and ultimately converges to the high probability density areas. This method helps to transform some complex high-dimensional problems into simple low-dimensional ones.

The objectives of this study were to find the posterior distribution of ecotype-specific cultivar parameters by combining the MCMC method with a process-based wheat model (WheatGrow) developed by the authors' group (Cao and Moss, 1997; Yan et al., 2000; Lv et al., 2013), to validate the effect of the MCMC-based method for parameter estimation at site and regional scales, and to quantify the parameter uncertainty on phenology estimation at site and regional scales. The expected results may provide a technical basis for estimating ecotype-specific cultivar parameters and developing regional applications of crop simulation models.

2. Materials and methods

2.1. Selection of study regions

Based on the wheat sowing area of each county in China obtained from the statistical yearbook for 2005, we used the sowing-area-weighted method (Jagtap and Jones, 2002) to aggregate the data of county-level wheat sowing areas in 2005 to $0.5^\circ \times 0.5^\circ$ resolution grid-level value. We then calculated the ratio of the wheat sowing area to the total area in each grid (Fig. 1).

Four major wheat production provinces, the Jiangsu, Hebei, Henan and Shandong provinces, which have the largest wheat sowing fraction of land in China, were chosen as study regions. Within the study region, we selected four representative ecosites (represented as green stars in Fig. 1), Huai'an (119.02°, 33.4°), Zhengzhou (113.4°, 34.49°), Weifang (119.05°, 36.42°) and Shijiazhuang (114.38°, 37.53°), to calibrate and validate the ecotype-specific cultivar parameters at the site scale. We used 62 other ecosites (represented as green triangles in Fig. 1) for validation at the regional scale.

2.2. Data collection and processing

Daily meteorological data from 1980 to 2005 for our four representative ecosites, and from the 62 other ecosites from 2004 to 2005, were provided by the Chinese Meteorological Administration. The data included daily maximum and minimum temperatures, precipitation, and sunshine hours. The sunshine hours were converted to solar radiation using Pohlert's method (2004). The National Meteorological Center Library of China provided the historical measurements of phenological stages, (which included sowing, jointing, anthesis, and maturity in wheat crops) at the four representative ecosites from 1980 to 2005, as well as measurements from the 62 other ecosites from 2004 to 2005. The different cultivars planted at each ecosite from 1980 to 2005 were cultivars recommended in each province.

Since wheat phenology prediction and uncertainty analysis at the regional scale required daily meteorological data at each $0.1^\circ \times 0.1^\circ$ resolution grid, the thin-plate smoothing splines of Hutchinson (TPS), described in the ANUSPLIN software package version 4.3 (Hutchinson, 1995, 2004), were used to generate the interpolated daily meteorological surfaces for the study area. This was based on the meteorological data from 62 ecosites in the four Chinese provinces from 2004 to 2005. The raw data from Digital Elevation Model (DEM) provided by the Consultative Group on International Agricultural Research (New et al., 2002) were used to help generate interpolated daily meteorological data. A second-order spline was fit by using latitude, longitude, and ele-

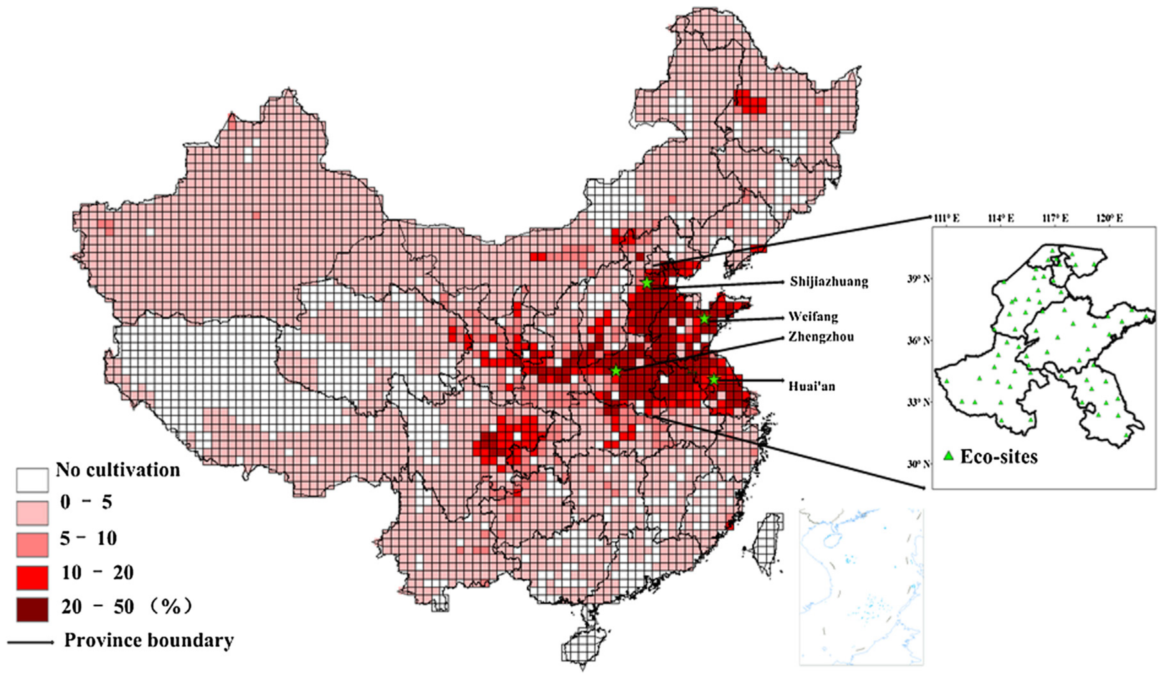

Fig. 1. Distribution map for proportion of wheat sowing area and selected ecosites in China. (Green stars and triangles represent 4 representative ecosites and 62 other ecosites, respectively.) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

vation as independent variables to interpolate the daily surfaces of maximum and minimum temperatures, and by using latitude and longitude as independent variables to interpolate the daily surfaces of precipitation and sunshine hours (Hutchinson, 2004).

2.3. Phenology model

The existing process-based model, WheatGrow, used for estimating wheat phenology in this paper was developed by the authors' group (Cao and Moss, 1997; Yan et al., 2000, 2001; Cao et al., 2003; Lv et al., 2013). In this model, the physiological development time (PDT) (Liu et al., 2000) was used as the development scale to predict the phenological development under various conditions. The interaction of daily thermal effectiveness [temperature sensitivity (TS) is included in this development process], daily thermal sensitivity [physiological vernalization time (PVT) and photoperiod sensitivity (PS) were included in this development process] and intrinsic earliness (IE) or basic filling duration factor (FD) determined the daily physiological effectiveness (DPE), which accumulated to account for the physiological development time (PDT). The PDT values of jointing, booting, heading, anthesis, initial filling and maturity stages were 16.1, 21.4, 26.8, 31, 39, and 56, respectively. The cultivar parameters in the model included TS, PVT, PS, IE and FD in relation to the development processes of wheat plants (Table 1). More details can be found in Supplementary material.

2.4. Method for estimating ecotype-specific cultivar parameters

The Markov Chain Monte Carlo (MCMC) technique, based on the Bayesian approach, can effectively synthesize information from various sources to analyze model uncertainties and optimize model parameters (Ceglar et al., 2011). Based on the existing model for estimating wheat phenological stages and by using the MCMC technique, a corresponding method was develpoed to estimate the posterior probability distribution of ecotype-specific cultivar parameters for the development stages of wheat at the four ecosites: Huai'an, Zhengzhou, Weifang and Shijiazhuang in China. Three important phenological stages (jointing, anthesis and maturity) from 1980 to 1995 were chosen for model calibration. The details of the Bayesian probability inversion and MCMC techniques have been described by Tao et al. (2009).

The posterior probability is proportional to the prior distribution times the likelihood $\pi_p\left(\theta\right)$. The prior distribution reflects our current knowledge of the parameters. When limited information is available, Van Oijen et al. (2005) suggested the use of uniform distributions, bounded by a biophysically or biologically reasonable maximum and minimum value for each parameter. The prior distributions in our study (Table 1) were set to uniform distribution, bounded by a maximum and minimum value for each parameter.

The likelihood function used in MCMC techniques has a very strong influence on parameter estimation. Several studies (He et al., 2010; Xu et al., 2006) have been carried out to simplify the likelihood function. In our study, three important phenological stages were chosen (i.e., yearly observation of jointing, anthesis and maturity dates). The model errors (the differences between simulations and observations) were assumed to follow a multivariate Gaussian distribution with a mean of zero. This assumption has been made in many other studies (Braswell et al., 2005; Tao et al., 2009; Xu et al., 2006). Because the model errors are not independent, correlations between the model errors arose when several measurements were performed at different dates in a given site-year (Makowski et al., 2006). There was no evidence of correlation between the model errors obtained in different years in our study. It seems reasonable to estimate only the covariances between model errors obtained in the same year and to set the other covariances to zero. Based on the Ternary Gaussian distribution (Sheng et al., 2008) at *t* time and considering correlations between above the above three phenological stages, the likelihood function was calculated at all observation times as follows:

$$\pi_p\left(\theta\right) \propto \exp\left\{-\left(\frac{1-\rho_{23}^2}{\sigma_1^2\times\alpha}x_1^2+\frac{1-\rho_{13}^2}{\sigma_2^2\times\alpha}x_2^2+\frac{1-\rho_{12}^2}{\sigma_3^2\times\alpha}x_3^2+\frac{2\left(\rho_{13}\rho_{23}-\rho_{12}\right)x_1x_2}{\sigma_1\sigma_2\times\alpha}\right.\right.$$
$$\left.\left.+\frac{2\left(\rho_{12}\rho_{23}-\rho_{13}\right)x_1x_3}{\sigma_1\sigma_3\times\alpha}+\frac{2\left(\rho_{12}\rho_{13}-\rho_{23}\right)x_2x_3}{\sigma_2\sigma_3\times\alpha}\right)\right\} \quad (1)$$

Table 1
Cultivar parameters related to estimation of phenological stages in WheatGrow model.

Parameter	Range of parameter	Definition	Unit
PVT	[0–60]	Physiological vernalization time is vernalization days requirement	Day
PS	[0.00–0.012]	Photoperiod sensitivity is the sensitivity for a cultivar to the photoperiod	–
IE	[1–3]	Intrinsic earliness is the fastest growth rate without the limitations of vernalization and photoperiod	–
TS	[0–2]	Temperature sensitivity is the sensitivity for a cultivar to the temperature	–
FD	[0–1]	Filling duration factor reflects the length of filling duration	–

$$\alpha = 1 + 2\rho_{12}\rho_{13}\rho_{23} - \rho_{13}^2 - \rho_{12}^2 - \rho_{23}^2 \quad (2)$$

$$\rho_{xy} = \frac{\sum_{t=1}^{15}(x_t - \bar{x})(y_t - \bar{y})}{\sqrt{\sum_{t=1}^{15}(x_t - \bar{x})^2}\sqrt{\sum_{t=1}^{15}(y_t - \bar{y})^2}} (x, y = 1, 2, 3) \quad (3)$$

$$x_j = \sum_{t=1}^{15}\left[O_j(t) - S_j(t)\right]^2 (j = 1, 2, 3) \quad (4)$$

where σ_1, σ_2 and σ_3 were the standard deviations of model errors (the differences between simulations and observations) at the jointing, anthesis and maturity dates, respectively, for the past 15 years; $S_j(t)$ and $O_j(t)$ were estimated and observed values respectively; j = {1, 2, 3} represented the jointing, anthesis and maturity dates, respectively; ρ_{xy} and $\bar{x}$ represent the correlation coefficients and the average of the model errors, respectively, of different phenological stages for the past 15 years; x_t and y_t represent the model errors of the different phenological stages at the *t* year.

2.5. Development of a system for estimating ecotype-specific cultivar parameters

The input data for the system for estimating ecotype-specific cultivar parameters includes latitude, longitude, daily maximum and minimum temperatures, precipitation, sunshine hours, observed phenological stages, and the arbitrary initial parameters for phenological development in wheat. The output data were stored in an access database, including the likelihood values $\pi_p(\theta)$, estimated phenology stages, and sampling results of cultivar parameters at each ecosite.

2.6. Evaluating the MCMC-based method for estimating ecotype-specific cultivar parameters

At the site scale, three phenological stages (jointing, anthesis and maturity) from the years 1996–2005 were used to evaluate the MCMC-based method at the four representative ecosites (green stars in Fig. 1). 1000 random parameter sets were randomly sampled from the prior and posterior parameter distributions at each ecosite separately, and calculated the jointing, anthesis and maturity dates. The mean of the estimations based on 1000 sets of parameters at each ecosite, combined with the observed values from 1996 to 2005 at each ecosite, were used to evaluate the MCMC-based method by calculating the R^2 and the root mean square error (RMSE) between observed and estimated values at the site scale. The uncertainty of phenology estimation was evaluated at the site scale using root mean square deviation $\left(\overline{RMSD}\right)$.

At the regional scale, the data from 62 other ecosites (green triangles in Fig. 1) in the four provinces from 2005 were used to evaluate the MCMC-based method. The ecotype-specific cultivar parameters were assumed to be valid for the whole province. The optimal 50 sets of parameters that produced the minimum RMSE between estimated and observed phenology from 1980 to 1995 were chosen from the 1000 parameter sets of the posterior parameter distributions. The optimal 50 sets of parameters from Huai'an, Zhengzhou, Shijiazhuang and Weifang represented ecotype-specific cultivar parameters of the Jiangsu, Henan, Hebei and Shandong provinces, respectively. The mean of the estimations based on the 50 sets of parameters at each ecosite, combined with the observed values of jointing, anthesis, and maturity dates, were used to evaluate the MCMC-based method at the regional scale by calculating the R^2 and RMSE between the observed and estimated values. Uncertainties in phenology prediction at the regional scale were evaluated by using RMSD. First, the TPS method was used to interpolate the daily weather data of the 62 other ecosites (green triangles in Fig. 1) in the four provinces from 2004 to 2005 to the daily weather data of 5202 grids at a resolution of $0.1^\circ \times 0.1^\circ$. Then, the phenological development model was run grid by grid, and the estimation results as 50 sets of parameters × 5202 grids × 1 year = 260,100 sets of simulation results were obtained. Finally, the estimated values of 5202 grids at $0.1^\circ \times 0.1^\circ$ resolution were used to calculate the RMSD at the regional scale and the mapping of RMSD.

R^2, RMSE and $\overline{RMSD}$ at site and regional scales were used to evaluate the MCMC-based method for estimating ecotype-specific cultivar parameters, in which R^2 and RMSE represented the fitness between the observed and estimated phenological stages, and $\overline{RMSD}$ represented the dispersion among estimated values, respectively. The RMSE and $\overline{RMSD}$ can be calculated according to Eqs. (5)–(8).

$$RMSE = \sqrt{\frac{\Sigma_{j=1}^{N}(O_j - \bar{S}_j)^2}{N}} \quad (5)$$

$$\bar{S}_j = \frac{1}{K}\sum_{i}^{K} S_{i,j} \quad (6)$$

$$\overline{RMSD} = \frac{1}{N}\sum_{j=1}^{N} RMSD_j \quad (7)$$

$$RMSD_j = \sqrt{\frac{\Sigma_{i=1}^{K}(S_{i,j} - \bar{S}_j)^2}{K}} \quad (8)$$

where N and K represent the total number of the year and random parameter set, respectively; O_j and $\bar{S}_j$ represent the observed and the estimated phenological stages in the *j* year, respectively; $S_{i,j}$ was the *i*th member of estimated phenology in the *j* year, and $RMSD_j$ was the root mean square deviation in the *j* year.

3. Results

3.1. Estimation of ecotype-specific cultivar parameters

Three parallel chains were made by the MCMC method, and each chain was simulated 60,000 times. Convergence of parallel chains was monitored using Gelman-Rubin (G-R) statistics for each parameter GR_i (Gelman and Rubin, 1992). The idea of the G-R test was that if the simulated Markov chain reached convergence, the within-run variation should be roughly equal to the between-run variation. The value of $GR_i \le 1.2$ was used as a standard indicator of convergence (Iizumi et al., 2009). In our case, approximately

Table 2
The mean values, standard deviations, and 95% confidence intervals of the posterior probability distribution of each parameter at four ecosites.

Ecosite	Parameter	95% credible interval	Mean value	Standard deviation
Huai'an	PVT	[4–51]	22	14.6
	PS	[0.0057–0.0092]	0.0079	0.0011
	IE	[1.08–1.98]	1.47	0.28
	TS	[0.088–1.05]	0.52	0.31
	FD	[0.49–0.70]	0.59	0.067
Zhengzhou	PVT	[10–56]	31	14.31
	PS	[0.0066–0.0098]	0.0086	0.001
	IE	[1.46–2.71]	2.04	0.38
	TS	[0.064–1.39]	0.6	0.4
	FD	[0.49–0.77]	0.61	0.089
Weifang	PVT	[5–53]	35	14.94
	PS	[0.0082–0.011]	0.0097	0.00073
	IE	[1.46–2.38]	1.72	0.27
	TS	[0.094–1.10]	0.54	0.32
	FD	[0.58–0.84]	0.7	0.083
Shijiazhuang	PVT	[10–53]	40	13.3
	PS	[0.0078–0.011]	0.0098	0.00076
	IE	[1.32–2.18]	1.86	0.25
	TS	[0.033–0.48]	0.23	0.14
	FD	[0.57–0.77]	0.66	0.064

50,000 iterations were required to reach the specified precision ($GR_i \leq 1.2$). The acceptance rates for the newly generated samples were about approximately 33–42% for the three chains. The initial number of samples in the burn-in period (10,000 samples) was discarded, and 50,000 samples from the final chain were used to calculate the means, variance and 95% confidence intervals for the posterior probability distribution.

Ecotype-specific cultivar parameters are defined as a probability distribution, not just specific values. Table 2 shows the means, standard deviations, and 95% confidence intervals of the posterior probability distribution of each parameter at the four ecosites. The posterior distributions of the parameters differed between the four ecosites. The mean value of PVT in Shijiazhuang was 40, the largest value among the four ecosites, with the lowest value of 22 in Huai'an. The mean value of PS ranged from 0.0079 in Huai'an to 0.0098 in Shijiazhuang. The mean value of TS ranged from 0.23 in Shijiazhuang to 0.6 in Zhengzhou. The mean value and standard deviation of IE in Zhengzhou were both larger than those at the other ecosites. The mean value of FD ranged from 0.59 in Huai'an to 0.7 in Weifang. The ranges of the posterior parameter were narrower than the prior parameter ranges.

Fig. 2 shows the posterior probability distribution of five parameters at four ecosites. The posterior probability distributions at the four ecosites differed from each other because of the distinct "ecotype" cultivars grown in each region. The order of estimated values of PVT and PS with highest probability among the four different ecosites was 46 and 0.00102 (Shijiazhuang), 38 and 0.001 (Weifang), 32 and 0.0092 (Zhengzhou), and 12 and 0.0083 (Huai'an). The estimated peak values of FD among four different ecosites were 0.67 (Weifang), 0.63 (Shijiazhuang), 0.58 (Huai'an), and 0.57 (Zhengzhou). The order of estimated IE with highest probability among four different ecosites was 2.0 (Zhengzhou), 1.81 (Shijiazhuang), 1.71 (Weifang), and 1.32 (Huai'an). The estimated TS with the highest probability at Weifang was higher than those at the other three ecosites, suggesting that wheat in Weifang was more sensitive to temperature.

3.2. Validating the MCMC-based method for parameter estimation at site and regional scales

3.2.1. Validating the MCMC-based method for parameter estimation at the site scale

Fig. 3 shows the observations and estimations based on 1000 sets of parameters from the posterior distributions at Huai'an, Zhengzhou, Weifang and Shijiazhuang from 1996 to 2005. The R^2 and RMSE between the observations and the means of the estimations based on 1000 parameter sets from the posterior distributions for three main phenological stages are summarized in Table 3. The R^2 was greater than 0.61 at the four ecosites, whereas the RMSE was less than 3.61 days. The R^2 ranged from 0.66 at Shijiazhuang to 0.72 in Zhengzhou for the jointing date, from 0.62 in Shijiazhuang to 0.72 in Zhengzhou for the anthesis date and from 0.61 in Shijiazhuang to 0.64 in Weifang for the maturity date. Among the three main phenological stages, all the R^2 values for jointing date at four ecosites (with the exception of Huai'an) were the highest, followed by the anthesis and maturity dates. In contrast, the RMSEs varied from 2.22 days in Weifang to 3.61 days in Huai'an for the jointing date, from 2.03 days at Weifang to 3.47 days in Zhengzhou for the anthesis date and from 2.07 days in Weifang to 2.82 days in Zhengzhou for the maturity date. All of the RMSE values for maturity at the four ecosites were lower than for the other phenological stages with the exception of Weifang (Table 3). The ecosites in Weifang and Shijiazhuang (both at a higher latitude) had relatively lower RMSEs for the three main phenological stages than did those in Huai'an. These results indicate that the phenological stages of wheat could be estimated reliably using the MCMC method.

The degree of model updating was evaluated from prior to posterior distributions by calculating R^2, and RMSE (Table 3). All R^2 values for the three phenological stages obtained by using the posterior probability distribution were higher than those based on the prior probability distribution at the four ecosites, with the exception of the anthesis date in Zhengzhou. However, R^2 was not improved appreciably except for the three phenological stages in Huai'an. Calibration tended to remove only the parameter sets with the poorest output-data correlation. All of RMSE values for the three phenological stages obtained using the posterior probability distribution at the four ecosites were significantly lower than those based on the prior probability distribution. The MCMC-based method significantly reduced the differences between simulations and observations.

3.2.2. Validating the MCMC-based method for parameter estimation at the regional scale

Fig. 4A, B and C shows the average estimates based on 50 parameter sets at each grid for the jointing, anthesis and maturity dates, respectively, for 2005. The estimated phenology was later in the higher latitude than in the lower latitude regions, and the three main phenological stages exhibited the same trend. Fig. 5 shows the scatter plots of the observed and estimated three main phenological stages at the 62 ecosites in the four provinces. The R^2 ranged from 0.86 to 0.93, and the RMSE ranged from 3.1 days to 3.4 days among the three different phenological stages. The R^2 and RMSE, respectively, were 0.93 and 3.4 days for the jointing date, 0.89 and 3.1 days for the anthesis date and 0.86 and 3.3 days for the maturity date. The highest R^2 and RMSE values were observed for the jointing date, while the lowest R^2 and RMSE values were observed for the maturity and anthesis dates, respectively.

3.3. Uncertainty in phenology prediction

3.3.1. Uncertainty in phenology prediction at the site scale

The dispersion of estimates in Fig. 3 indicates the uncertainty of the phenology estimation derived from the uncertainty of the

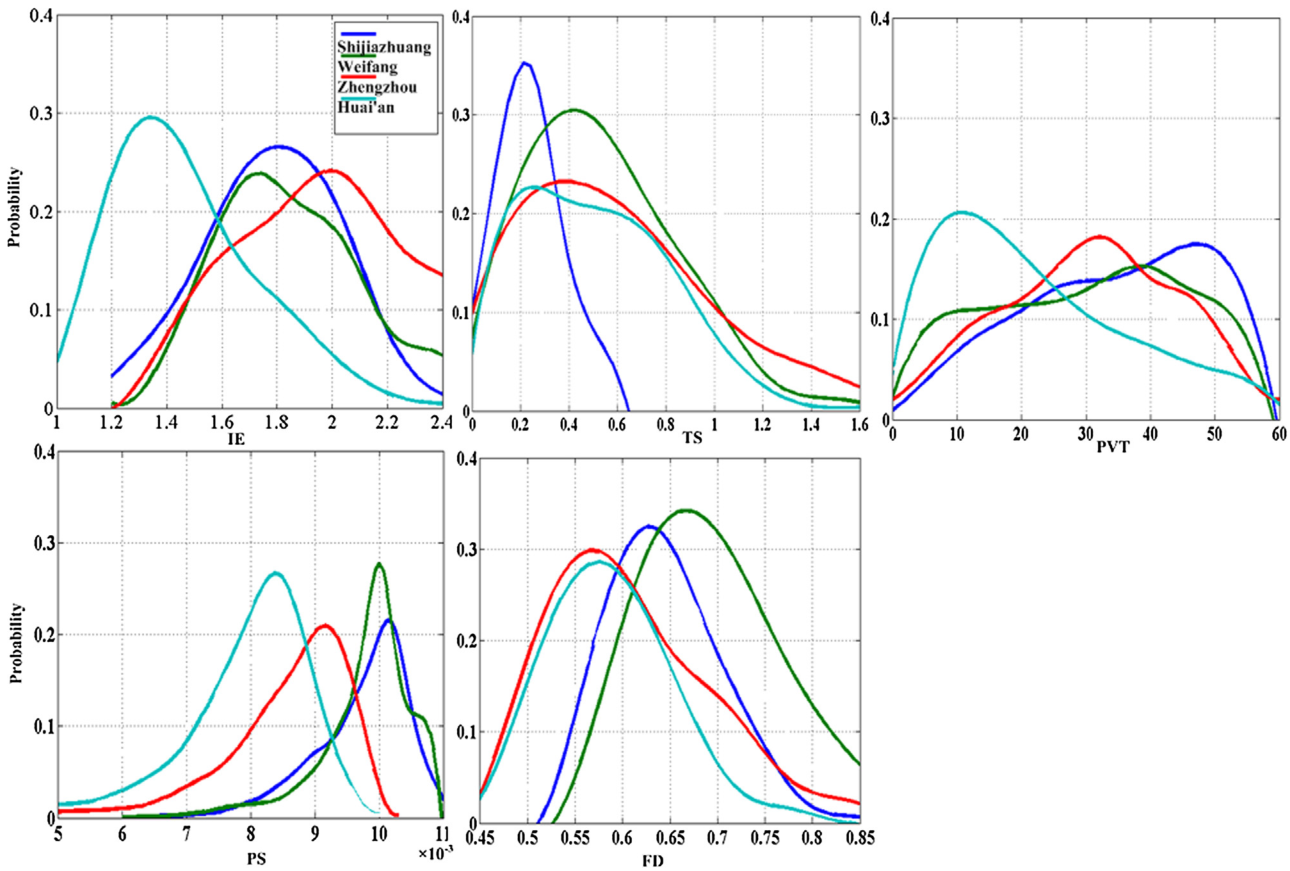

Fig. 2. Posterior probability distribution of five ecotype-specific cultivar parameters at four ecosites.

Table 3
The R^2, RMSE and $\overline{\text{RMSD}}$ at site scale were used to evaluate the MCMC-based method for prior and posterior parameter distributions.

Site		Jointing			Anthesis			Maturity		
		R^2	RMSE (day)	$\overline{\text{RMSD}}$ (day)	R^2	RMSE (day)	$\overline{\text{RMSD}}$ (day)	R^2	RMSE (day)	$\overline{\text{RMSD}}$ (day)
	Prior	0.09	7.53	7.51	0.39	8.48	6.09	0.39	6.58	5.51
Huai'an	Posterior	0.69	3.61	4.00	0.70	2.65	3.61	0.62	2.38	3.27
	Prior	0.71	8.12	8.62	0.78	4.83	6.30	0.5	7.26	5.93
Zhengzhou	Posterior	0.72	3.13	3.83	0.72	3.47	3.47	0.59	2.82	3.22
	Prior	0.62	8.31	6.19	0.60	6.47	6.51	0.53	5.03	5.96
Weifang	Posterior	0.69	2.22	3.48	0.66	2.03	3.53	0.64	2.07	3.24
	Prior	0.64	8.72	6.63	0.40	7.77	6.69	0.52	6.79	6.45
Shijiazhuang	Posterior	0.66	2.35	3.32	0.62	2.61	3.45	0.58	2.14	3.20

parameters. The 10-year averages of $\overline{\text{RMSD}}$ based on 1000 parameter sets from the posterior distributions for the three main phenological stages are summarized in Table 3. The $\overline{\text{RMSD}}$s ranged from 3.32 days in Shijiazhuang to 4.00 days in Huai'an for the jointing date, from 3.45 days in Shijiazhuang to 3.61 days at Huai'an for the anthesis date and from 3.20 days in Shijiazhuang to 3.27 days in Huai'an for the maturity date. All of the values of the $\overline{\text{RMSD}}$s for the maturity date at the four ecosites were lower than for the other phenological stages (Table 3). The ecosites in Weifang and Shijiazhuang (at higher latitude) had relatively lower $\overline{\text{RMSD}}$ values for the three main phenological stages than those in Huai'an and Zhengzhou.

Fig. 3 shows predictive uncertainty before and after calibration for the three phenological stages. Model output uncertainties based on posterior probability distributions were greatly reduced compared to the prior distribution. All of the $\overline{\text{RMSD}}$ values for three main phenological stages obtained using the posterior probability distribution were lower than those based on the prior probability distribution (Table 3). The correlations between prior and posterior $\overline{\text{RMSD}}$ for the three phenology stages in Huai'an, Zhengzhou, Weifang and Shijiazhuang were 0.98, 0.96, 0.90 and 0.95, respectively.

3.3.2. *Uncertainty in phenology prediction at the regional scale*

Fig. 4D, E, and F display the corresponding RMSD values of the jointing, anthesis and maturity dates for 2005 at $0.1^\circ \times 0.1^\circ$ resolution. The RMSD for the jointing date was relatively higher than for the anthesis and maturity dates. Almost all the RMSDs at the grid scale were less than 4 days for the jointing date, and were less than 3 days for the anthesis and maturity dates. The RMSDs in Fig. 4D, E and F indicated the uncertainty of the phenology estimation when the phenology model was extended to the regional scale. The mean ± the RMSD (Fig. 4) at each grid reflects 68.27% confidence intervals for the regional wheat phenology forecast.

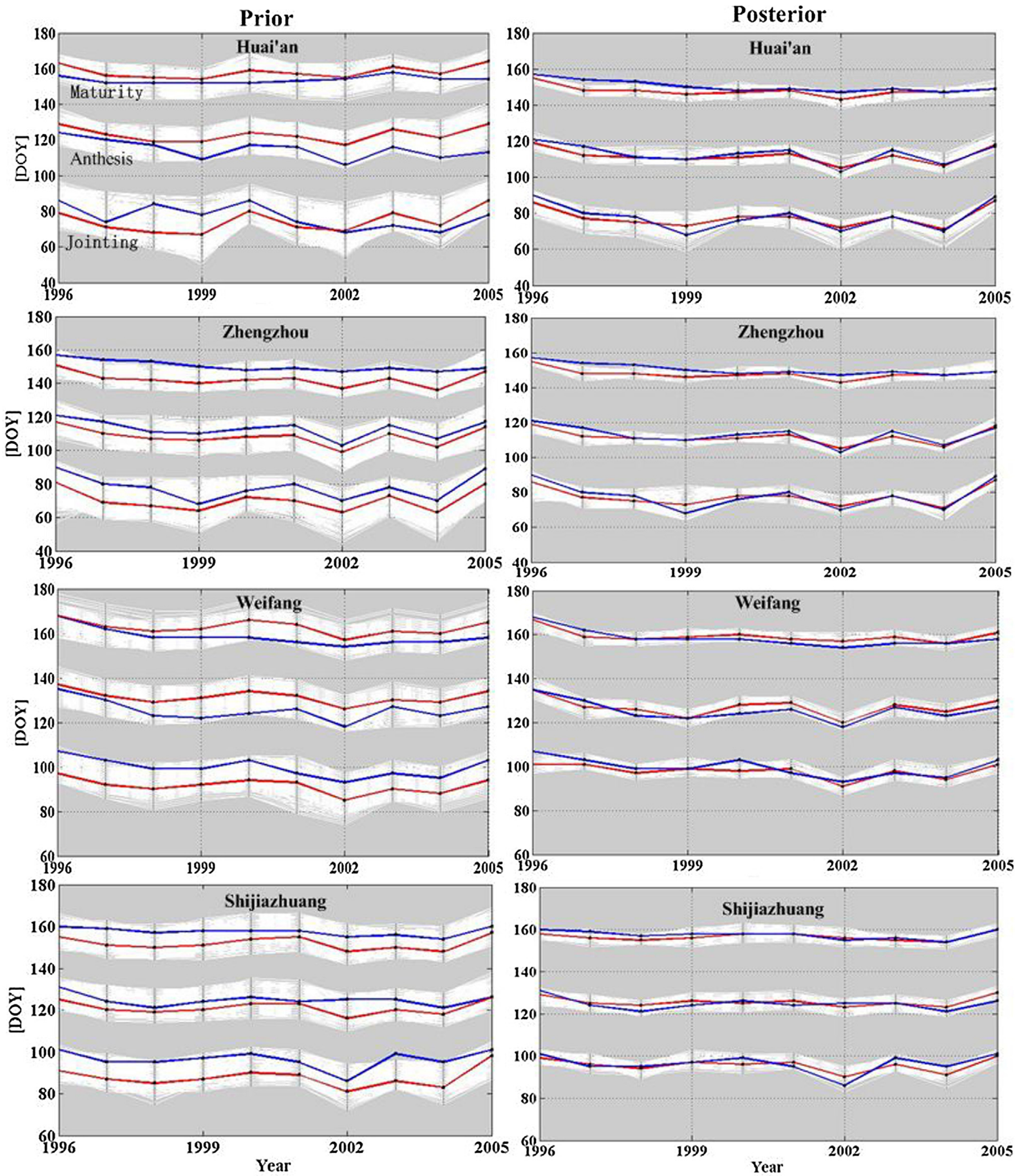

Fig. 3. The observations and estimations based on prior and posterior parameter distributions regarding jointing, anthesis and maturity dates at four ecosites from 1996 to 2005. Blue line: observations, red line: the mean of estimations based on 1000 parameter sets, thin white line: estimations based on 1000 parameter sets. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. Discussion

4.1. MCMC method for parameter estimation

Through the global sensitivity analysis method (linear regression), Duan (2011) analyzed the parameter sensitivity of the WheatGrow model and found that the most sensitive parameters for the anthesis and maturity dates were, successively: TS, PVT, PS, IE, and FD. The other parameters, such as the thresholds of PDT values, Tb, To, and Tm, have little influence on phenology. Therefore, TS, PVT, PS, IE and FD were taken as a subset while the other parameters were taken as fixed values. If all the parameters were used for calibration, computational load may increase and parameters convergence may be affected (Minunno et al., 2013). The results of our study suggest that a subset of the parameters of the model did not affect the model performance. Many studies (Van Oijen et al., 2011;

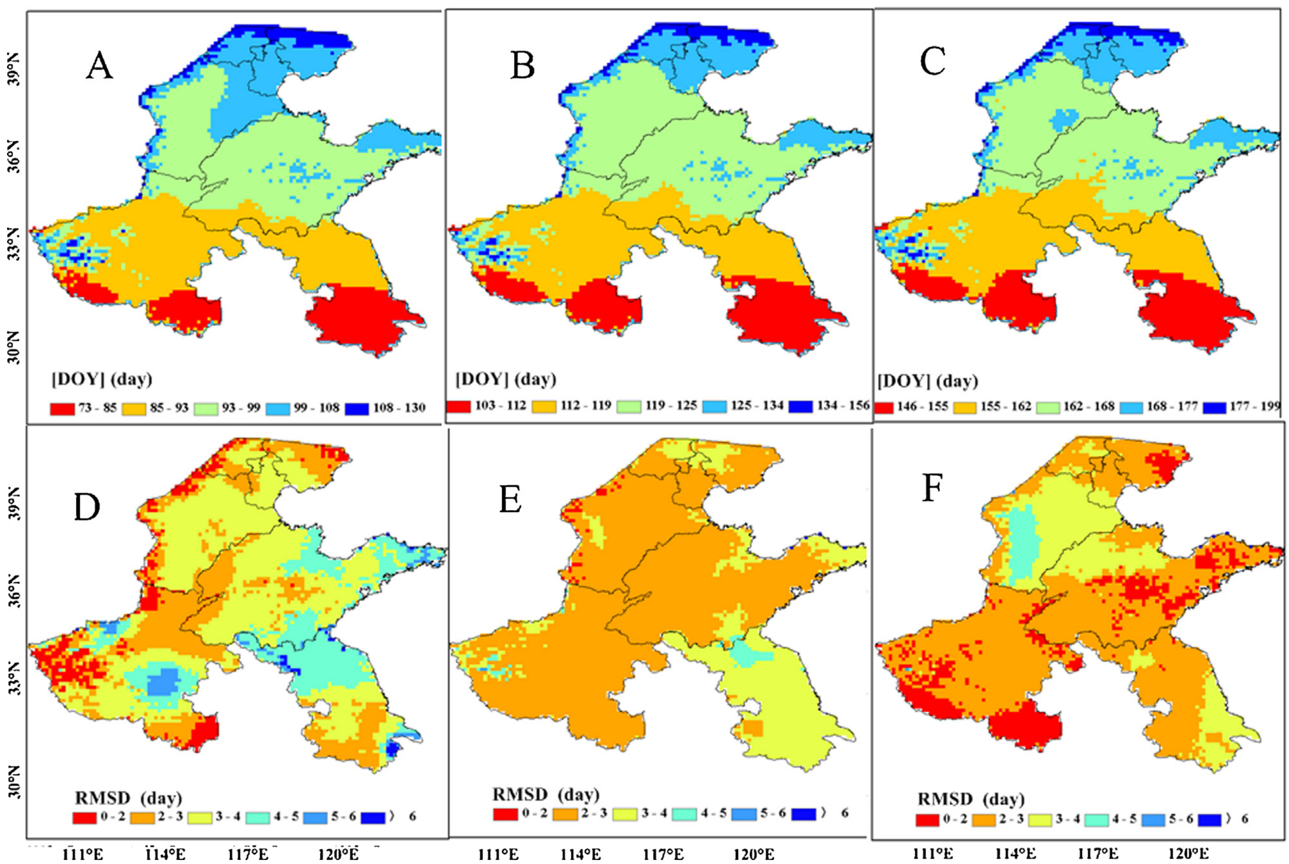

Fig. 4. Spatial patterns of estimations (A, B, C) and RMSDs (D, E, F) for jointing, anthesis and maturity dates of wheat in four provinces in the wheat growing season for 2005.

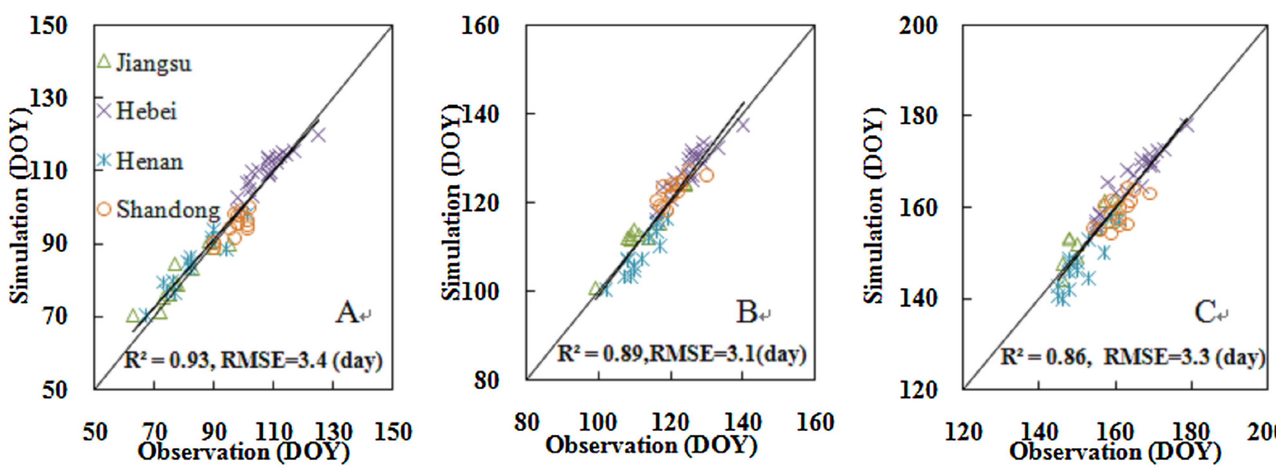

Fig. 5. Scatter plots of the estimated and observed values for three phenological stages in the wheat growing season for 2005 at 62 ecosites in four provinces ((A) jointing; (B) anthesis; (C) maturity).

Minunno et al., 2013) also used a parameter subset, instead of the full parameter set, for Bayesian calibration of complex models.

Traditional methods of parameter estimation have aimed at finding an optimal set of parameter values within some particular model structure (Mertens et al., 2004). These methods often present a partially rather than globally optimal combination of model parameters and cannot help us understand uncertainties in the parameters and how those uncertainties affect predictions (He et al., 2009). Bayesian methods can greatly improve the accuracy of model predictions. Compared to the Generalized Likelihood Uncertainty Estimation method (GLUE), the values of mean squared error from model predictions are slightly lower with the MCMC method than with the GLUE method (Makowski et al., 2002). Furthermore, the MCMC method has exhibited powerful capabilities to reduce uncertainties in parameters and predictions in complex models (Van Oijen et al., 2013).

The likelihood function used in the MCMC technique had a very strong influence on parameter estimation. Some researchers (Xu et al., 2006; He et al., 2010) only considered one or two phenological stages when constructing the likelihood function. Additionally, many studies have been carried out to simplify the likelihood function. Wallach (2006) constructed the likelihood function with three types of measurements, and did not consider the covariances between model errors of the same type of measurement at different

Table 4
Correlations between model errors of jointing, anthesis and maturity stages.

Eco-sites	r_1	r_2	r_3
Huai'an	0.47	0.05	0
Zhengzhou	0.51	0.17	0.47
Weifang	0.14	0.10	0.64
Shijiazhuang	0.28	0.19	0.16

Note: r_1 was the correlation of model errors between jointing and anthesis; r_2 was the correlation of model errors between jointing and maturity; r_3 was the correlation of model errors between anthesis and maturity.

dates in a given site-year. Tao et al. (2009) also constructed a likelihood function for phenology without considering the covariances between model errors. Model errors obtained in a given site-year are often correlated. We constructed the likelihood function for wheat phenology and took full account of the covariances between different dates in the same year because there were large interactions between different phenological stages in the same year (Table 4). To study the structure of the model errors, the differences between observations and estimations were calculated for different phenological stages for 1980–2005. As shown in Table 4, all correlations between model residuals were above 0 at the four ecosites, and some correlations were even above 0.5. Model errors obtained in a given site-year are often correlated. For example, when a model overestimates one phenological stage at a certain site-year, it is likely that other phenological stages are overestimated at different dates. Thus, not only the three main phenological stages but also the interactions between model errors of different phenological stages in the same year were considered when constructing the likelihood function, which ensured the accuracy of phenology estimation for the whole growth period. However, there was no evidence of correlation between the model errors obtained in different years in our study. Thus, it seems reasonable to estimate the covariances between the model errors obtained only in the same year and for the same type of measurement, with the other covariance values set to zero.

4.2. Regional difference in posterior distribution

The ranges of the posterior parameters were typically narrower than the prior parameter ranges, suggesting that the MCMC-based method reduced the uncertainty of the parameters. However, not all parameters exhibited a significant reduction. The posterior distribution of PVT at the four ecosites did not show a very clear peak and remained spread across their prior range of variation (Fig. 2). This is because there was interaction between the vernalization progress and the photoperiod effectiveness (Ream et al., 2014). Full vernalization is not required for flowering under effective photoperiods (Cao and Moss, 1997). For example, some winter wheat sowed in spring can also flower under effective photoperiods. Therefore, PS may compensate for PVT under specific photoperiod conditions.

PVT and PS reflect vernalization day requirements and the sensitivity to the photoperiod for a cultivar, respectively. The order of estimated PVT and PS with highest probability among the four different ecosites was consistent with the actual situation. Winter wheat planted at high latitudes requires more days to finish vernalization than that at low latitudes (Cao and Wu, 2000). Cao and Moss (1997) also proved that photoperiod sensitivity was higher for the cultivars planted at high latitudes than for those planted at low latitudes. FD reflects the length of filling duration. The estimated FD with highest probability among the four different ecosites decreased as the mean value of actual grain filling period from 1980 to 1995 increased: Weifang (32.5 days), Shijiazhuang (32.56 days), Huai'an (35.16 days), and Zhengzhou (35.6 days). Liu et al. (2000) proved that the FD was negatively correlated with the length of the grain filling period. In general, the posterior distribution of

Table 5
The correlation coefficients of five ecotype-specific cultivar parameters based on 50,000 sets of parameter of the final chain at four ecosites.

Site		PVT	PS	IE	TS	FD
Huai'an	PVT	1				
	PS	−0.67	1			
	IE	−0.021	0.11	1		
	TS	0.18	−0.52	0.66	1	
	FD	0.11	−0.51	0.23	0.74	1
Weifang	PVT	1				
	PS	−0.55	1			
	IE	−0.18	0.67	1		
	TS	−0.05	−0.1	0.45	1	
	FD	−0.05	−0.14	−0.18	0.4	1
Zhengzhou	PVT	1				
	PS	−0.36	1			
	IE	0.11	0.084	1		
	TS	0.069	−0.63	0.61	1	
	FD	0.025	−0.62	0.33	0.85	1
Shijiazhuang	PVT	1				
	PS	−0.53	1			
	IE	−0.17	0.32	1		
	TS	−0.01	−0.41	0.6	1	
	FD	−0.02	−0.34	0.027	0.6	1

the ecotype-specific cultivar parameters quantified by MCMC was consistent with our observations.

In our research, the phenological development of wheat was affected by the vernalization progress, the photoperiod effectiveness progress and the thermal effectiveness progress. There were interactions between these progresses (Rahman, 1980; Davidson et al., 1985; Trevaskis et al., 2007; Herndl et al., 2008). For example, wheat displays a wide range of flowering responses to various photoperiods and lengths of vernalization (Ream et al., 2014). Meanwhile, there were interactions between different parameters (Table 5). The effects of some parameters may compensate under specific climate conditions for each other (e.g. photoperiod sensitivity and vernalization requirements) so that many different combinations of parameter values can produce very similar results. For example, two sets of parameters (PVT, PS, IE, TS and FD were values of 10, 0.0073, 1.35, 0.81 and 0.66, respectively, for cultivar A and 44 0.0047, 1.35, 0.81 and 0.66, respectively, for cultivar B) estimated in Huai'an produced similar phenological stages. Of these five parameters, only PVT and PS are different. If cultivar B planted in Huai'an does not finish vernalization, phenological development will be adjusted by photoperiod effectiveness. However, the cultivars that are well adapted to specific climate conditions in the growing region should typically have quite similar responses to temperature and photoperiod (Cao and Wu, 2000). Cultivar A may be well adapted to the climate conditions in Huai'an, while cultivar B may be adapted to other regions. Therefore, the "true" range of the parameters should in practice be much narrower than the parameter range in the posterior probability distribution (Fig. 2). The ecotype cultivars corresponding to the posterior probability distribution of parameter values should include the "true" ecotype-specific cultivars planted in each province, the cultivars not planted in each province and the cultivars that may not exist. Since the parameter distributions were unknown, we set the prior distributions as uniform distributions and ensured that they were wide enough to cover a very wide range of possible values. For further research, 95% confidence intervals of the posterior probability distribution for each parameter at the four ecosites may be taken as the prior probability distribution.

4.3. Uncertainty in phenology prediction

The uncertainty of phenology estimation derived from the uncertainty of the parameters, as seen in Table 3, and in Figs. 3 and 4, indicates that the uncertainties of phenology estimation changed over time at the site scale and from one gird to another at the regional scale. The integration of Bayesian probability inversion and the MCMC technique is an effective method to analyze the uncertainties in parameter estimation and model prediction. Many studies have quantified the uncertainty of phenology estimation at the site scale. Ceglar et al. (2011) used different phenological methods for estimating the development rate of maize, and quantified the uncertainties of maize phenology estimation. He et al. (2009) estimated the genetic parameters of the CERES-Maize model in DSSAT with the GLUE method and assessed the uncertainties of maize phenology. In this study, the uncertainties of wheat phenology estimation were quantified not only at the ecosites of Shijiazhuang, Zhengzhou, Huai'an and Weifang but also in the four provinces at the regional scale.

Fig. 4 shows the apparent differences for RMSD values among the provinces. The correlations between site and region RMSD for jointing, anthesis and maturity dates in the year 2005 were 0.83, 0.73 and 0.51, respectively. The uncertainties of phenology estimation at the regional scale were associated with optimized parameters at the site scale. In the same province, the same ecotype-specific parameters were used to evaluate the uncertainty of the phenology estimation, but the RMSDs differed for different grids. Therefore, the uncertainty of the phenology estimation at the regional scale not only came from the uncertainty of the optimized parameters at the site scale, but also from spatial differences in climate. Our research only showed the regional uncertainty of phenology estimation only for 2005, which is a limitation of the study regarding the regional uncertainty estimates. In addition, we assumed that the ecotype-specific cultivar parameters were the same within a province. Due to data limitations, we did not calibrate the parameters for every grid. Although the parameters that determine the phenological characteristics probably have little or no scale dependency (Iizumi et al., 2014), we did not know the scale ranges for ecotype-specific cultivar parameters in our research. Therefore, the relationship between parameter values and the spatial scale should be studied in further research.

5. Conclusion

The MCMC-based method was used for phenological estimation at four ecosites, namely Huai'an, Shijiazhuang, Zhengzhou and Weifang in the main wheat growing regions of China. This method produced reliable results for the posterior distributions of the ecotype-specific cultivar parameters. The ranges of the posterior parameters were narrower than the prior parameter ranges. The estimated phenology with 1000 sets of parameters agreed well with the observed phenology at the site scale. When going from prior to posterior distributions, all of RMSE and $\overline{\text{RMSD}}$ values for the three phenological stages obtained using the posterior probability distribution at the four ecosites were significantly lower than the prior probability distribution. The extension of the ecotype-specific cultivar parameters demonstrated that the estimated parameters were also applicable at the regional scale. The estimated phenology was consistent with the actual phenology for 2005. The uncertainty of phenology estimation in the growing season for 2005 was quantified with the RMSD in large regions. Overall, the present MCMC-based technique exhibited high reliability for estimating ecotype-specific cultivar parameters in our wheat simulation model, and should provide a useful basis for extending the crop simulation model from a field simulation to regional application.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.agrformet.2016.02.016.

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