Evaluation of a regional climate model for impact assessment of climate change on crop productivity in the tropics

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Regional climate models (RCMs) are considered to be more useful than general circulation models for assessing impacts of climate change scenarios in agriculture. In this communication, the climatic outputs of an RCM–PRECIS (providing regional climates for impact studies) model were analysed by comparing its baseline simulation daily weather data on temperature and precipitation patterns with the observed weather for the corresponding period (1960–1990) in order to find out the bias in the model. Results showed that model could simulate the mean weather parameters on an aggregated scale, but could not satisfactorily represent spatio-temporal variations. There exists a bias towards higher precipitation along with more intense warm and cold events in the baseline simulation. In order to quantify the impacts of the PRECIS model biasness in baseline simulations on crop performance, rice (*kharif* season) and wheat (*rabi* season) yields were simulated using the observed weather and the PRECIS baseline weather for several locations representing the Indo-Gangetic Plains. With more extreme weather parameters in the baseline simulated data, the grain yields of rice and wheat were reduced, even causing wheat crop failure in several years as against none observed. The results indicated that using PRECIS baseline daily weather may cause bias in crop performance assessments. Since the bias in baseline will be carried forward in the assessment of future climatic impacts, there is a need to develop more reliable regional climate scenarios for the Indian region.

Keywords: Climate change, crop yield, impact assessment, regional climate models.

CLIMATE change is projected to have significant effects on agriculture production and hence on food security. The rising temperatures, carbon dioxide levels and uncertainties in rainfall associated with global warming may have serious direct and indirect impacts on crop production[1]. A loss of 10–40% crop production is predicted in India by the end of this century[2,3]. Temperatures exceeding the optimal level for biological processes cause a steep drop in net growth and yield[4]. Production of annual crops will be affected globally by the expected increase of 2–4°C in mean temperatures towards the end of the 21st century[5].

Climate change is projected to decline the yields of several major crops in India if no measures are taken[6–10]. Wheat is the major *rabi* crop in India and is sensitive to various biotic and abiotic stresses like weather and inter-seasonal climate variability[11]. Simulation studies using InfoCrop model showed that the current wheat production in India may decrease with each degree increase in temperature above the current mean temperatures[12]. Simulated rice yields in Asia will also decrease by 7% for every 1°C rise above the current mean temperature[13]. In India, results have shown that a 2°C increase in mean air temperature could decrease rice yield by about 0.75 tonne/ha in the high-yield areas and by about 0.06 tonne/ha in low-yield coastal regions[14]. In fact, in North India, rice yields during the last three decades have shown a declining trend and this is possibly related to increasing temperatures[15]. Recent analysis has indicated spatial and temporal variation in the climate change impacts on irrigated and rainfed rice yields[9]. Most of the results about the impacts of climate change in tropical developing countries of Asia and Africa are based on global climate model (GCM) outputs. However, there are relatively few studies in the tropics where regional climate models (RCMs) have been used for assessing agricultural impacts. For large countries with diverse climate and agricultural practices such as India, it becomes important that assessments are done using RCMs[8–10].

Assessments of the vulnerability of crops to the changing climate are based on the estimates of the impacts of climate change in the given scenarios of future climate. These scenarios are largely designed from GCMs. Even though climate variations and changes may be partly predictable, particularly on the larger (e.g. continental, global) spatial scales, there are significant differences at the regional levels[16]. These GCM projections may be adequate up to a few 100 km or so; however, they do not capture the local details often needed for impact assessments at a national and regional level. To systematically pursue such assessments, the most fundamental requirement is the availability of reliable estimates of future climatic patterns on the regional scale, which can be readily used for impact assessment. RCMs, have the potential to improve the representation of the climate information, which is important for assessing vulnerability to climate change over smaller regions[17].

However, it is important to understand the model bias in the GCMs and RCMs before impact assessments are made. In this communication, we present the analysis on climatic outputs of PRECIS (providing regional climates for impacts studies) – an RCM having HadCM3 (UKMO GCM) climate inputs[18]. Further, a crop simulation model

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(InfoCrop) was used to quantify the impact of model bias on simulated yield of rice and wheat. The specific objectives of this study are to: (i) evaluate the suitability of PRECIS baseline-derived daily weather data on temperature and precipitation patterns with actual measured data in different locations in India, and (ii) compare the crop yield simulated by InfoCrop model using observed weather and RCM baseline weather for rice and wheat in the Indo-Gangetic Plain (IGP) region, the food basket of India.

Twenty-three locations representing diversity in major crop-growing areas and climatic patterns in India were selected for this analysis. The critical climatic parameters such as rainfall, maximum and minimum temperature for the past 30 years at these locations were compared with the PRECIS simulated baseline values for the corresponding period (1961–1990). Observed weather and baseline weather were then used to simulate the crop yield using InfoCrop, a generic crop simulation model.

PRECIS is a simplified version of the GCM HadCM3 developed by the Hadley Centre, United Kingdom[17]. PRECIS can be run on a PC and can be applied easily to any area of the globe to generate detailed climate change predictions. This RCM has a high resolution of 50 km and can be applied to any area of the globe to generate detailed climate change scenarios. PRECIS provides daily weather data for 30 years period of 1960–1990 as the baseline and also future scenarios. The simulated parameters are over Indian domain at surface level (56.77–103.233E, 1.503–38.23N) with a horizontal resolution of 0.44° × 0.44°. The model output consists of various surface as well as upper air parameters such as precipitation, maximum and minimum temperature, surface radiation, relative humidity, wind speed, etc.

The RCM baseline and observed daily data on these three weather variables for 30 years were analysed to calculate the following parameters, which could be used as indicators of climatic risks. (i) Annual and seasonal (*kharif* and *rabi*) means of maximum and minimum temperatures. (ii) Annual and seasonal (*kharif* and *rabi*) rainfall. (iii) Average number of rainy days (rainfall >2.5 mm/day) on seasonal (*kharif* and *rabi*) and annual basis. (iv) Intensity of rainfall (total rainfall/number of rainy days) on seasonal (*kharif* and *rabi*) and annual basis. (v) Average number of rainy days with >15 and >50 mm/day rainfall. (vi) Average number of days with >40°C, >45°C mean maximum temperature in a year. (vii) Average number of days with <20°C mean maximum temperature in a year. (viii) Average number of days with <5°C mean minimum temperature. (ix) Coefficient of variation of rainfall and maximum and minimum temperature.

Model bias was calculated by comparing the mean and extreme events in weather parameters in RCM baseline weather data with the observed weather. If the baseline values are higher than the observed maximum temperatures, then the model is considered to have bias towards high temperature. If the minimum temperatures are lower than the observed values, then it is considered as bias towards low temperature. Similar criteria were followed while analysing rainfall patterns and extreme events.

InfoCrop is a generic crop growth model that can simulate the effects of weather, soil, agronomic managements (including planting, nitrogen, residue and irrigation) and major pests on crop growth and yield[19]. The model considers different crop development and growth processes influencing the simulation of yield. The total crop growth period in the model is divided into three phases, viz. sowing to seedling emergence, seedling emergence to anthesis and storage organ filling phases. The model requires various varietal coefficients, viz. thermal time for phenological stages, potential grain weight, specific leaf area, maximum relative growth rate and maximum radiation use efficiency. The model requires crop management inputs such as time of planting, application schedule and amount of fertilizer and irrigation, soil input data such as soil pH, soil texture, thickness, bulk density, saturated hydraulic conductivity, soil organic carbon, slope, soil water-holding capacity and permanent wilting point. Location-wise daily weather data (solar radiation, maximum and minimum temperature, rainfall, wind speed, vapour pressure) are also required to simulate crop performance.

InfoCrop considers the processes of growth and development, soil water, nitrogen and carbon, and crop–pest interactions. Each process is described by a set of equations, the parameters of which vary depending upon the crop/cultivar.

- Crop growth and development: phenology, photosynthesis, partitioning, leaf area growth, storage organ numbers, source–sink balance, transpiration, uptake, allocation and redistribution of nitrogen.
- Effects of water, nitrogen, temperature, flooding and frost stresses on crop growth and development.
- Crop–pest interactions: damage mechanisms of insects and diseases.
- Soil water balance: root water uptake, inter-layer movement, drainage, evaporation, runoff, ponding.
- Soil nitrogen balance: mineralization, uptake, nitrification, volatilization, inter-layer movement, denitrification, leaching.
- Soil organic carbon dynamics: mineralization and immobilization.
- Emissions of greenhouse gases: carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O).

Calibrated and validated InfoCrop – wheat and rice models were used to simulate the yields using observed weather data and simulated baseline data for the 30 year period (1960–1990). Nine representative locations in the Indo-Gangetic area, which is a major rice and wheat-growing

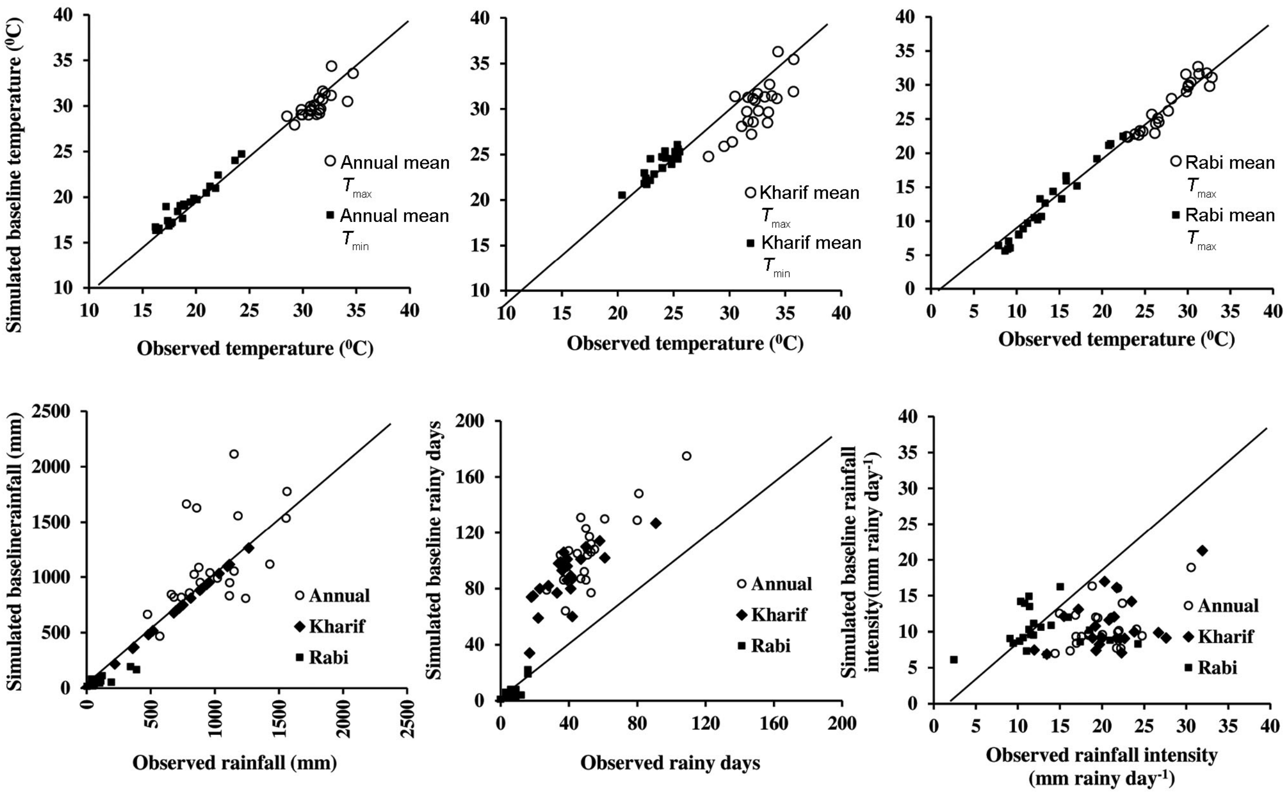

Figure 1. Comparison of PRECIS simulated baseline climate with observed climate (1961–1990) in 23 locations representing spatial variation in different climatic condition across India. Each data point represents mean of 30 years (1961–1990) for each location.

area were selected. These were Ludhiana, Hisar, Karnal, Saharanpur (upper IGP), Pantnagar, Lucknow, Varanasi (middle IGP), Patna and Barrackpore (lower IGP). The wheat crop was sown in the second week of November, whereas rice was transplanted in the first week of July. Crop was managed by providing fertilizer @ 120 kg N in two splits for wheat and @100 kg N in three splits for rice in water non-limiting conditions. Yield thus obtained was compared by frequency distribution analysis.

The annual mean minimum temperature was slightly overestimated by the RCM baseline across the country ranging from 0.02°C to 0.5°C, except for central India where the model slightly underestimated the mean minimum temperatures by 0.07–0.9°C. On the other hand, RCM baseline mean maximum temperatures were less than the observed values in the respective locations (Figure 1), indicating a bias towards cool temperature ranging from 0.24–2.36°C in the model. Results could not indicate any spatial trend in this bias. A similar study conducted in Bangladesh using PRECIS also reported the systematic cold bias in simulating the annual scale of the surface temperature, where the model underestimated the temperature by about 0.61°C within a range +1.45°C to –3.89°C in different months[20]. Considering the small deviation from the observed, it can be concluded that PRECIS adequately simulated the spatial variation in annual temperature across India.

The lowest and highest rainfall areas of RCM baseline almost matched with the observed rainfall (Figure 1). However, rainfall was therefore overestimated in parts of North India, central and south central India. The model bias ranged from +34% to –89% of annual rainfall across India, indicating poor performance of the model in simulating the baseline rainfall patterns. The PRECIS model simulated more rainy days in the baseline period than those observed (Figure 1). The overestimation in the number of rainy days varied from 24 to 84 (60–200%) without any spatial pattern in the bias. Since the model simulated more rainy days, the annual rainfall intensity was found to be lower than that observed. The PRECIS model underestimated the rainfall intensity by 2–15 mm/rainy day and simulated rainfall also varied with that observed in different regions of China[21]. A better simulation was observed for precipitation in the north of China and in winter than in the south of China and in summer; simulated precipitation values were lower than those observed over the southeast coastal areas.

Analysis of the seasonal mean temperatures revealed that the model underestimated temperature. In *kharif* season, the baseline mean minimum temperatures followed the annual pattern of underestimation in central India, with overestimation for rest of the country. The range of underestimation was 0.11–1.56°C, whereas overestimation ranged from 0.27°C to 0.93°C. However, mean

Table 1. Comparison of the number of days with extreme weather parameters in observed (1961–1990) and RCM simulated baseline for the same period (each value represents the mean of 30 years)

			Number of days with									
			T_{max} > 45°C		T_{max} < 20°C		T_{min} < 5°C		Rainfall > 15 mm		Rainfall > 50 mm	
Location	Latitude	Longitude	Current	PRECIS BL	Current	PRECIS BL	Current	PRECIS BL	Current	PRECIS BL	Current	PRECIS BL
Tanjore	10°47′N	79°10′E	0	0	0	0	0	0	22	4	4	0
Coimbatore	11°00′N	77°00′E	0	0	0	0	0	0	10	1	2	0
Aduthurai	11°1′N	79°32′E	0	0	0	0	0	0	22	5	5	0
Kasargod	12°30′N	75°00′E	0	0	0	0	0	0	61	98	21	3
Dharwad	15°27′N	75°05′E	0	0	0	0	0	0	14	4	2	0
Hyderabad	17°20′N	78°30′E	0	3	0	2	0	0	19	13	2	3
Cuttack	20°28′N	85°54′E	1	15	0	3	0	2	17	26	3	3
Junagadh	21°31′N	70°36′E	0	1	0	0	1	0	14	40	3	4
Indore	22°44′N	75°50′E	1	11	1	4	1	3	18	16	4	2
Barrackpore	22°45′N	88°26′E	0	4	2	17	0	8	33	30	7	2
Bhopal	23°16′N	77°36′E	0	11	2	14	0	20	23	33	5	3
Ranchi	23°23′N	85°23′E	0	6	6	29	7	32	33	26	6	2
Patna	25°00′N	85°00′E	0	13	6	64	3	28	22	14	5	1
Varanasi	25°20′N	83°00′E	1	25	9	63	2	30	20	12	4	0
Gwalior	26°14′N	78°10′E	0	21	8	45	20	51	17	16	4	0
Lucknow	26°76′N	80°87′E	1	20	11	78	8	45	17	12	3	1
Delhi	28°38′N	77°12′E	3	22	33	75	24	62	15	10	3	0
Pantnagar	29°03′N	79°31′E	0	15	19	63	18	50	26	15	8	1
Hisar	29°10′N	75°7′E	3	0	26	64	46	71	9	6	1	0
Karnal	29°70′N	76°9′E	0	21	47	79	17	71	12	9	2	1
Saharanpur	29°00′N	77°00′E	0	20	23	73	21	72	22	9	6	1
Ludhiana	30°90′N	75°8′E	1	29	42	78	31	74	14	7	3	1

BL, Baseline.

minimum temperatures during *rabi* season were underestimated in most places by 0.27–3.21°C, indicating a strong bias towards lower or cooler days in the model.

In case of seasonal mean maximum temperature, PRECIS baseline simulations underestimated the values in *kharif* by 0.32–4.92°C, while in *rabi*, the range was 0.11–3.24°C. Results indicated that, in general, PRECIS underestimation of seasonal mean maximum temperatures was more during *kharif* than *rabi*. On the other hand, the biasness on mean minimum temperature was more during *rabi* than in *kharif* season. In central and south central India, the underestimation for mean maximum temperatures during *kharif* ranged from 3°C to 4.9°C, while that during *rabi* in North India ranged from 1.5°C to 3.21°C. From the findings of a similar type of study conducted on the annual cycle in the surface air temperature on all-India basis, cold bias to certain extent was reported in the PRECIS model throughout the year, particularly in the seasons other than spring[16].

Most parts of India receive monsoon-dependant rainfall, which occurs during *kharif* season amounting to about 89% of the annual rainfall. In the season-wise rainfall pattern, the model overestimated the *kharif* rainfall in most parts of the country. On the other hand, the *rabi* rainfall was underestimated. Observed rainfall in *rabi* season was only about 11% compared to *kharif* in most of the places in the country, except in the southwest regions of Tamil Nadu, where bimodal rainfall exists. Apart from the overestimation of *kharif* rainfall and underestimation of *rabi* rainfall, the PRECIS model was also unable to simulate the bimodal rainfall pattern. Previous studies[2] on the spatial patterns of seasonal rainfall as simulated by PRECIS for the baseline period, in comparison with the observed as well as the driving global models HadCM3 and HadAM3, also showed the existence of some quantitative biases. They reported that the conspicuous bias was considerably higher than observed monsoon precipitation over east central India in the baseline simulation and concluded that the regional model inherits some of the biases in the driving global model since they found this bias in HadAM3 also.

Simulated number of rainy days had overestimation trends in seasonal (*kharif* and *rabi*) and annual scale. However, in South India, differences in observed and simulated rainy days in baseline period were found to be less. Due to more simulated rainy days in *kharif*, there was a corresponding discrepancy with the observed patterns. The rainfall intensity differences up to 18.49 mm rainy day^{-1} from observed to baseline values were found in the north Indian locations; model was simulating lower intensity of rainfall. Compared to the *kharif* rainy day simulations, the model performance in simulating *rabi* rainy days was satisfactory, even though simulated baseline rainfall intensity was less than that observed.

The robustness of model in representing the extreme events of temperature and precipitation was evaluated in different locations, since these events are most prominently seen in smaller spatio-temporal scales. Only a few locations in North India were found to have maximum temperature of more than 45°C for 1–3 days period in a year, but RCM simulated baseline indicated days with a maximum temperature of 45°C and above in most parts of India, other than the locations in South India. The number of days was significantly higher than that observed, even more than 20 days in some locations. In some locations nearly 25% of these hot days were in the *kharif* season (Table 1). Similarly, central and northern India had more number of days with <20°C as the maximum temperature; however, the model overestimated the number of cooler days in all locations. Similar patterns were observed for the number of days with 5°C or less as the minimum temperature. The model was found to have a bias towards both extremes of temperature, thus simulating more number of hot as well as cold events, especially over central and northern India. Earlier analysis indicated that PRECIS model had simulated considerably more intense warm and cold events over large parts of north India[16]. As far as rainfall intensity is concerned, PRECIS in general underestimated the rainy events of >15 and 50 mm/day. However, in a few locations the model overestimated the events with 15 mm or more rainfall ranging from 9 to 37 days. This clearly indicated that the model could not simulate the rainfall extremes properly.

Coefficient of variation analysis indicated that the PRECIS model could not capture the observed inter-annual variability across locations, particularly for mean maximum temperature and annual rainfall (Figure 2). Even though the inter-annual variability could be simulated in areas having more homogenous years, for areas with higher variability the model simulated baseline could not represent the same. Overall results indicate that PRECIS model had significant biases in simulated baseline values, which become significant in impact assessments, particularly in the agricultural sector.

In order to quantify the impacts of PRECIS model bias in baseline simulations on crop performance, rice (*kharif* season) and wheat (*rabi* season) yields were simulated using the observed weather and the PRECIS baseline weather for locations representing the IGP. In rice, the average simulated yield using observed weather varied from 5068 to 5657 kg/ha in various locations. When RCM baseline data were used, a similar range was noticed (4946–5546 kg/ha). The frequency distribution analysis of rice yield (Figure 3) showed that in the upper and middle IGP, simulated yields using RCM data followed a similar pattern as simulated yields using observed weather data. However, in general the yields in RCM baseline were lower than those observed. On the whole, in RCM baseline many years were in the low yield range and few years were in the higher range compared to those observed. In the upper, middle as well as lower IGP, the same trend was observed. Even with the overestimation of *kharif* rainfall in the RCM baseline, the rice yields were not significantly affected because waterlogging does not affect crop growth under water non-limiting conditions. During *kharif* season, more hot days were found in the baseline weather where the minimum temperatures were also higher than the observed weather and this high temperature period coincided with the sensitive stages of the crop such as flowering and grain filling, resulting in lower yield. The high temperature during the developmental stage of the crop has an important effect on the damage experienced by the plant[22] and the negative effects of high temperature tend to be larger for grain yield than for total biomass[23,24]. The temperatures encountered during flowering can result in a reduction in a

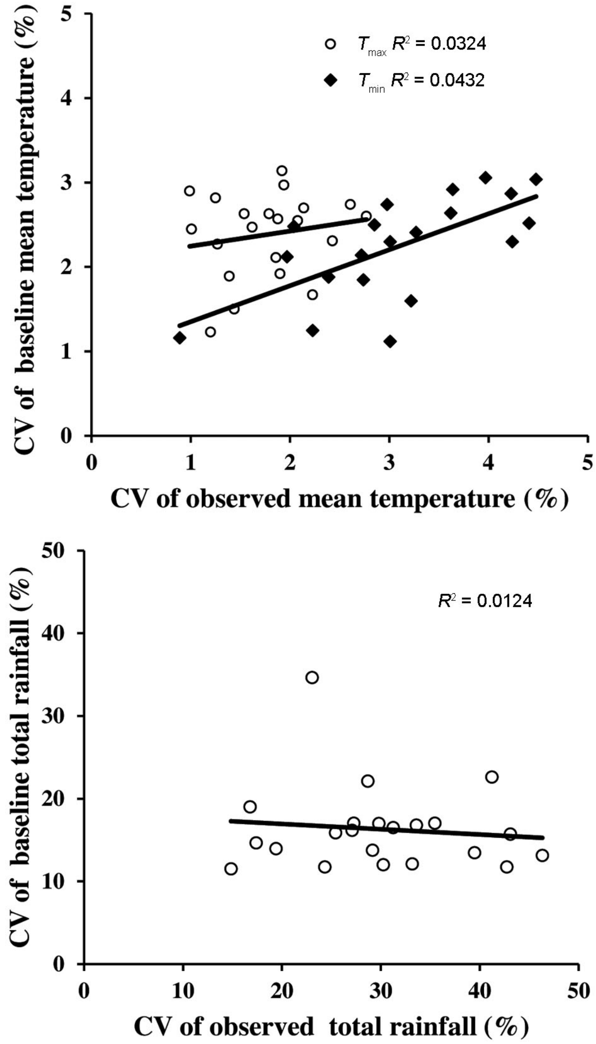

Figure 2. Coefficient of variation (CV) in the observed and PRECIS baseline weather parameters in 23 locations representing spatial variation in different climatic condition across India. Each data point represents mean of 30 years (1961–1990) for each location.

yield, in spite of any lengthening of duration in rice[25]. Results showed that bias of RCM weather data reflected on lowering the yield output of rice crop.

In the case of wheat, the average yield ranged between 4275 and 4871 kg/ha when simulated using observed weather. However, because of too many cold events in the baseline weather in some locations, crop failure occurred and hence the simulated average yield varied between 973 and 4237 kg/ha. The frequency distribution analysis (Figure 4) showed that in the IGP region nearly 25% of the years faced crop failure while in the other years very low yield was observed when simulated using PRECIS baseline weather. This was more prevalent in the upper IGP region followed by the middle and lower IGP regions. When RCM baseline was used in the upper IGP area nearly 56% of the years faced crop failure, whereas in middle IGP it was for about 23% of years. In both these regions more number of years were in low yield range. However, in the lower IGP region no crop failure was simulated. Analysis of both past observed and PRECIS baseline weather data indicated model bias towards cold temperature. This led to greater number of cold and even frost days in most parts of the upper and middle IGP causing crop failure during *rabi* season. The frost days were observed during December and January coinciding with late tillering and panicle initiation stages, which are the most sensitive stages of wheat for low temperatures, and thus killed the crop in vegetative stage itself due to freezing injury[26–28]. In the case of wheat also, the model bias resulted in lowering the yields in a large number of years across the IGP. These results clearly demonstrate that the cold (during *rabi*) and hot (during *kharif*) biasness of PRECIS simulated baseline, reduced the yield performance of rice and wheat crops causing large number of years with lower yield than that simulated using observed weather.

The analysis further indicates that the baseline extreme events in low temperature severely affected the *rabi* crop growth (wheat) due to their coincidence with the crop growth period. But the baseline extremes in high temperature did not influence the *kharif* (rice) crop, as these events occurred during April and May. Generally the *rabi*

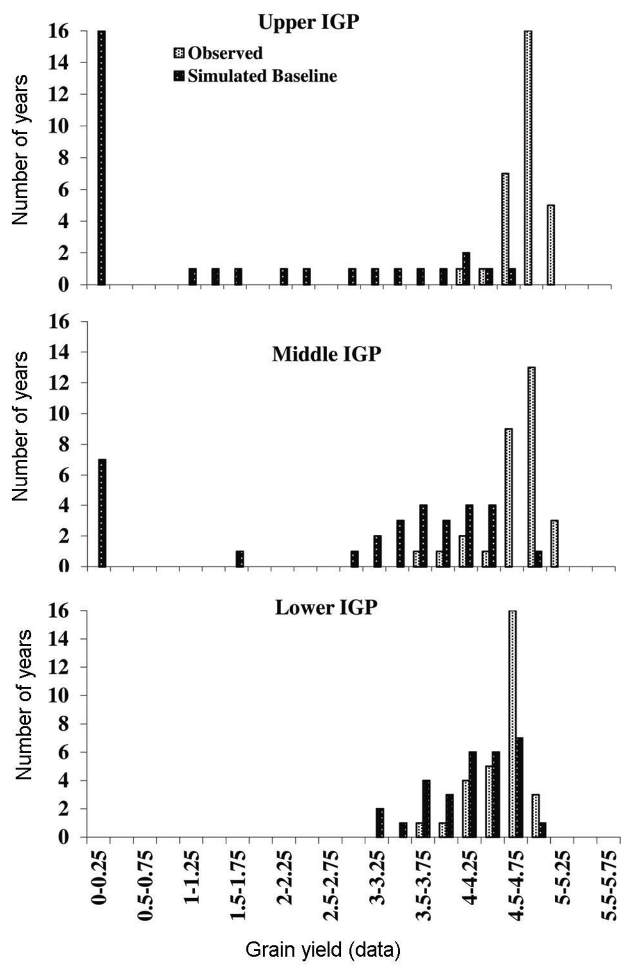

Figure 3. Comparison of frequency distribution of rice yield for 30 years using observed and PRECIS baseline weather in upper, middle and lower parts of the Indo-Gangetic Plains (IGP).

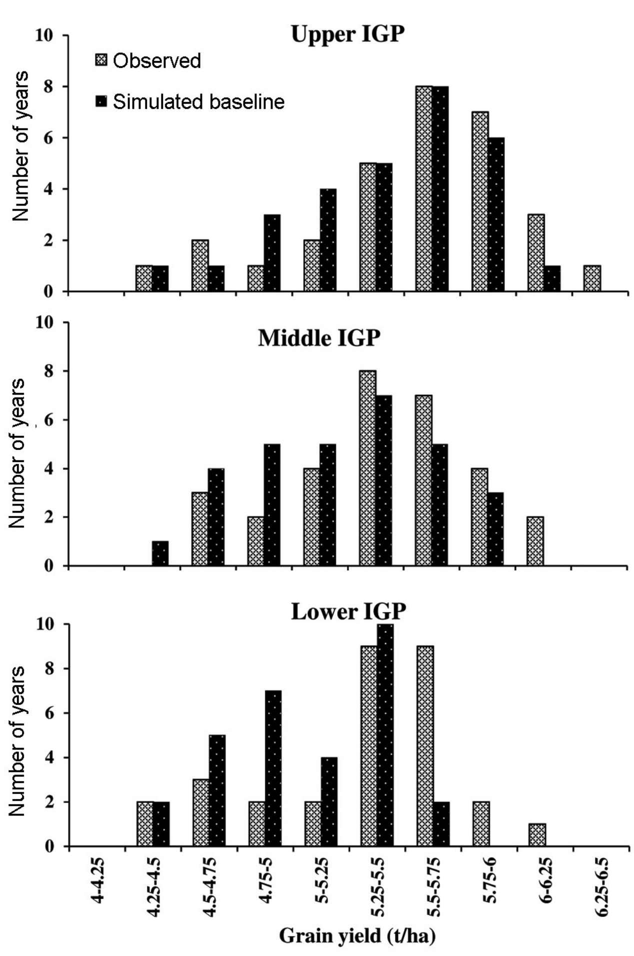

Figure 4. Comparison of frequency distribution of wheat yield for 30 years using observed and PRECIS baseline weather in upper, middle and lower parts of the IGP.

crops are harvested by March, while the *kharif* crop is sown from June onwards. However, high temperature bias will affect the analysis on summer season crops. As far as baseline extreme events in rainfall are concerned, the analysis on rice was not affected much due to the factors mentioned earlier. However, these biases in rainfall and temperature will adversely affect the analysis of rainfed crops and cross-pollinated crops by causing damage due to water stagnation, fertilization and seed set apart from other effects such as reduced phenology, increased senescence rate and reduced grain-filling period. Thus, the results indicate that the bias existing in the RCM model outputs adversely influence the crop model simulation analysis.

The RCMs are increasingly being used to capture the spatio-temporal variations in weather at regional as well as national level. The models bias increases from South to North India. Reports on satisfactory simulation of current climate using RCMs such as HadRM3H for most parts of the UK[29], CRCM for Canada[30], and HIRHAM4 model in Denmark[31] exist. However, PRECIS or HadRM3 does not satisfactorily represent the spatio-temporal variations in weather as observed. The models might have difficulty in capturing important topographical and physical processes responsible for temperature and precipitation patterns at regional scale. Similarly, PRUDENCE regional climate models for the British Isles reported that the RCMs are unable to simulate the spatial anomalies and as well as the observed frequency of drought events in their climate control, particularly for severe events, possibly due to a failure to simulate persistent low precipitation[32]. Apart from the above, the seasonal patterns for bias and variations in extreme events, as observed in this study, are also noted in HIRHAM model outputs. This suggests that not all RCMs are efficient in capturing the regional and temporal variations across the nation, particularly in countries with diverse environments such as India, and hence warrant more research to improve the model performance.

An evaluation of the PRECIS model by comparing observed precipitation and temperature patterns with those in the baseline simulation showed that the model could simulate the mean weather parameters on an aggregated scale, but could not satisfactorily represent spatio-temporal variations. These variations from observed weather became more biased with reduction in space and timescales, i.e. monthly and daily. There exists a bias towards higher precipitation along with more intense warm and cold events in the baseline simulation. This bias in the model may be inherited from its parent GCM. With more extreme weather parameters in the data, baseline weather was found to affect the simulated crop yields. Since the biases in baseline will be carried forward for assessment of future climatic patterns, there is a need for improvement in baseline simulations of PRECIS model for developing more reliable regional climate scenarios for the India.

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The influence of sugar–phosphate backbone on the stacking interaction in B-DNA helix formation

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The influence of sugar–phosphate backbone on the stacking interaction in the adenine…thymine base-pair dimer (A…T)$_2$ has been studied using the density functional theoretic method and the dispersion-corrected density functional BLYP-D3 and the triple-zeta quality basis set def2-TZVP. In the absence of the sugar–phosphate backbone, several stacked conformers were obtained with a small difference in their stabilization energy values (–20 to –25 kcal/mol). However, the presence of the sugar–phosphate backbone limits the movement of the two A…T units, and yet the stacking interaction remains significant (–19.4 kcal/mol). Despite the constraints imposed by the backbone, the dimer (A…T)$_2$ is found to retain its favourable geometry. The influence of sodium ions on the geometry and the interaction energy is found to be negligible.

Keywords: B-DNA helix formation, BLYP-D3, stacking interaction, sugar–phosphate backbone.

THE classic double-helical structure of B-DNA, proposed by Watson and Crick[1], is governed by hydrogen bonds between the Watson–Crick (WC) base pairs of anti-parallel strands, stacking interactions between nucleobases, and covalent bonds between the base pairs and the sugar–phosphate units[2–4]. The stabilization energy value associated with the stacking interaction between adenine, guanine, cytosine and thymine dimers ranges from 10 to 17 kcal/mol (ref. 3). In contrast, the strength of multiple hydrogen bonds between base pairs falls between 20 and 30 kcal/mol. Therefore, it can be concluded that the contribution of the stacking interaction to the overall stability of DNA is comparable to that of the hydrogen bonds. Although it is generally perceived that hydrogen bonding is primarily governed by electrostatic forces and π-stacking interaction by dispersion forces[4–7], in the recent past there have been instances where such perceptions have been challenged[8,9]. A recent molecular dynamics (MD) simulation study[10] showed that in the absence of the dispersion energy component, the double-helical structure is transformed into a straight ladder-like structure. The relative

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