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# Designing crop technology for a future climate: An example using response surface methodology and the CERES-Wheat model ☆

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## Abstract

Future crop production will be adapted to climate change by implementing alternative management practices and developing new genotypes that are adapted to future climatic conditions. It is difficult to predict what new agronomic technologies will be necessary for crop production under future climatic conditions. The purpose of this work was to develop an approach useful in identifying crop technologies for future climatic conditions. As an example of the approach, we used response surface methodology (RSM) in connection with the CERES-Wheat model and the HADCM2 climate simulation model to identify optimal configurations of plant traits and management practices that maximize yield of winter wheat in high  $CO_2$  environments. The simulations were conducted for three Nebraska locations differing in altitude and rainfall (Lincoln, Dickens and Alliance), which were considered representative of winter wheat growing areas in the central Great Plains. At all locations, the identified optimal winter wheat cultivar under high  $CO_2$  conditions had a larger number of tillers, larger kernel size, fewer days to flower, grew faster and had more kernels m<sup>-2</sup> than the check cultivar under

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normal  $CO_2$  conditions. In addition, optimal sowing dates were later and optimal plant densities were smaller than under normal conditions. We concluded that RSM used in conjunction with crop and climate simulation models was useful in understanding the complex relationship between wheat genotypes, climate and management practices. © 2005 Elsevier Ltd. All rights reserved.

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### 1. Introduction

The decision process of identifying new agronomic technology may be conceptualized as an optimization procedure. When developing new cultivars or new management practices, it is reasonable to assume that the major objective is to find the set of inputs, in this case the set of plant traits or management inputs or techniques, that result in a crop that optimizes (i.e., maximizes or minimizes) some response. The response to be optimized depends on the goal of the particular project, and may be a single variable, such as profit, yield, organic matter or runoff or some combination of variables. Most modern agronomic research is oriented toward identifying technologies that maximize profit. In many studies, field experiments are conducted under conditions similar to those that farmers would experience and results are used to make choices among possible technologies. Information about the best technologies is then either disseminated to farmers or incorporated into new research. While this classical agronomic research paradigm has been enormously effective in improving productivity and profitability in the last one-hundred and fifty years, this approach is not suitable for some problems.

One type of research that does not fit this classical research paradigm involves evaluating the possible long-term impacts of climate changes on agronomic technologies. This research can be useful in understanding the types of cultivars and management practices that may be necessary under likely future climates. It is generally not possible to conduct field experiments under future environmental conditions, nor is it simple to approximate the cumulative changes in technologies over a long period of time in response to climate change. Identifying technologies that may be necessary under future climates requires three components: (1) a method to generate or simulate future environmental and climatic conditions; (2) the ability to predict crop response under these future conditions and (3) an approach that approximates the decision process of identifying and selecting new agronomic technologies in response to climate change over a long period of time. Climate simulation models and crop growth and yield models have been used extensively to predict plant responses under future climatic conditions (Rosenzweig et al., 1995). However, no clear methodology has been proposed that simulates the long-term decision making process of identifying new agronomic technologies in conjunction with predicted plant responses under simulated future global climatic conditions.

Response surface methodology (RSM) used in connection with crop and climate simulation models can be adapted to approximate the long-term decision process of identifying future agronomic technology in response to climate change. RSM is an optimization approach commonly used in industrial process control and engineering where the goal is to find levels of input variables that optimize a particular response (Myers and Montgomery, 1995). RSM proceeds sequentially with a series of experiments to find the area near the optimal (maximum or minimum) response. A final experiment is then conducted to find the 'optimal' input combinations and to evaluate the nature of the surface in the area of the optimum. RSM is most useful when a response depends on many factors and the objective is to find the levels of these factors that give an optimum response. In addition, RSM is sequential in nature where current experiments are dependent upon predictions from previous experiments and thus is a reasonable approach to simulating human decision making over a long period of time. Other optimization procedures such as simulated annealing and genetic algorithms depend on random perturbations of the inputs and consequently are not reasonable approaches to modeling decision making processes. As a result, RSM can be a useful tool in approximating the long-term decision process of identifying new agronomic technologies in response to climate change.

As a simple example of how RSM might be used with crop and climate simulation models to approximate the process of identifying new technology, assume that a scientist would like to find levels of two inputs,  $X_1$  and  $X_2$  that maximize yield (y) of a particular crop in a particular climate. Further let yield be only a function of inputs  $X_1$  and  $X_2$  and a vector of climate related variables W or more specifically,  $y = f(X_1, X_2, W)$  where a simulation model quantifies this functional relationship. Also assume that  $X_1$  is a genetic trait such as kernel weight and  $X_2$  is a management variable such as planting density. A predicted yield value is generated for a particular set of inputs  $X_1$  and  $X_2$ , by simulating weather variables W for a future climate and using  $X_1, X_2$  and W in the crop simulation model to generate a yield. In a broad sense, RSM proceeds by sequentially adjusting  $X_1$  and  $X_2$  until maximum yield is achieved which approximates the scientist's search for improved cultivars and management practices.

In this simple example, the RSM procedure begins with an initial  $2 \times 2$  factorial first-order experiment, centered at the 'current' levels of  $X_1$  and  $X_2$  (point a in Fig. 1) where each of the four design points are identified by the levels of  $X_1$  and  $X_2$  in Fig. 1 and yield is measured on a third axis that is perpendicular to the  $X_1, X_2$  plane. Point a represents the current cultivar and management practice. At each of the four design points about a, yield values are simulated over a number of years and the across year mean yield (y) is obtained for each point. Based on these four y values, a first-order statistical model:  $y = b_0 + b_1X_1 + b_2X_2$  is fit to give a planar yield response surface as a function of  $X_1$  and  $X_2$ . Using this surface, the path of steepest ascent is determined as the line that predicts the steepest increase in yield (line ab in Fig. 1). Yield values are simulated sequentially at various  $X_1$  and  $X_2$  values along the path of steepest ascent until yield decreases substantially. Another  $2 \times 2$  factorial experiment is then conducted near the point of highest yield on the path of steepest ascent (point c, Fig. 1), another first-order statistical model is fit and a second path of



Fig. 1. Simple example of path of steepest ascent to identify maximum yield and optimal value for the two traits based on three computer simulation experiments.

steepest ascent is identified (line cd, Fig. 1). The process is continued until there is little increase in yield at which point a final second-order experiment is conducted to identify the values of  $X_1$  and  $X_2$  that maximize yield  $(X_{1,opt}; X_{2,opt} \text{ in Fig. 1})$ . This final experiment is normally a central composite design and data from this experiment are analyzed with a second-order model  $y = b_0 + b_1X_1 + b_2X_2 + b_{11}X_1^2 + b_{22}X_2^2 + b_{12}X_1X_2$ . Differentiating the estimated equation with respect to  $X_i$ , setting the result equal to zero and solving gives the optimal inputs,  $X_{i,opt}$ . Evaluation of the fitted response surface then determines the nature of the surface and the nature of the  $X_{i,opt}$  values, i.e., if they are maximum, minimum or saddle-points.

Ideally, the final values of  $X_{1,opt}$  (kernel weight) and  $X_{2,opt}$  (planting density) will maximize yield under the future climate scenario at this site. Even though the values of  $X_{1,opt}$  and  $X_{2,opt}$  are only based on simulations, they could be useful in understanding the types of cultivars and management practices that may be needed in future climates. Although this example is quite simplistic the method is quite general since any plant model with any number of input variables and any weather model can be used as long as the output (y), the inputs (X) and the weather variables (W) are clearly identified.

Climate models have predicted that in the next 100 years, the atmospheric concentration of  $CO_2$  could double and that temperature and precipitation patterns could change substantially (IPCC, 1995). The combined effect of these changes on winter wheat production is difficult to evaluate. Changes in temperature and precipitation patterns during critical periods of crop development can have dramatic positive or negative impacts while increases in  $CO_2$  concentration can raise the rate of photosynthesis, promoting biomass accumulation, increasing plant growth and yield (Kim-

ball, 1983; Cure and Acock, 1986). Whatever the climatic changes, crop production can be adapted to climate change by implementing alternative management practices and developing new genotypes that will take advantage of the future climatic conditions. However, these new agronomic technologies cannot be identified without understanding future climatic conditions that are likely to result. In addition, developing new cultivars will require knowledge of crop traits that will allow the crop to perform well in the future climate. Coupling response surface methods with crop and climate simulation models can be useful in understanding what types of cultivars and management practices may be necessary to maximize production in the future.

In this work, we used the CERES-Wheat model to simulate yield of wheat crops as a function of climatic variables, genetic coefficients, soil characteristics and management practices (Tsuji et al., 1994). CERES-Wheat, V3.0 (Ritchie and Otter, 1985) simulates daily growth and development of wheat as well as yield, has been validated for present  $CO_2$  and current climate conditions (Otter-Nacke et al., 1986), and has been widely used to assess wheat responses to elevated CO<sub>2</sub> and future climate change scenarios (Delecolle et al., 1995; Mearns et al., 1996; Rosenzweig et al., 1995; Tubiello et al., 1999; Weiss et al., 2003). The effect of increased CO<sub>2</sub> concentrations can be simulated by CERES-Wheat (Rao, 2002). The direct effect of increased CO<sub>2</sub> concentrations on growth responses in CERES-Wheat is achieved by multiplying the daily potential dry matter formed by a number (greater than one) that represents the ratio of the current to the future scenario carbon dioxide concentration. Tubiello et al. (1999) tested the modified CERES-Wheat model under elevated CO<sub>2</sub> treatments using field data from free-air carbon dioxide enrichment (FACE) experiments with spring wheat and found that simulations of dry matter and yield were, in most all cases, within 10% of measured values. For weather inputs of future climates, we used the LARS-WG V3.2 stochastic weather generator, to simulate appropriate weather data (Racsko et al., 1991; Semenov et al., 1998; Semenov and Brooks, 1999) based on a well-known climate model, the Hadley Center global climate model (HADCM2) (Johns et al., 1997). The objective of this research is to demonstrate the use of response surface methodology (RSM) with crop and climate models to identify optimal configurations of plant traits and crop management practices that maximize winter wheat yield under high CO<sub>2</sub> environments.

## 2. Materials and methods

CERES-Wheat was coupled with HADCM2 and RSM to identify levels of the non-weather CERES-Wheat input variables  $(X_i)$  that maximized yield under two CO<sub>2</sub>-weather scenarios (normal: 360 µmol/mol; high: 720 µmol/mol) at three Nebraska locations (Lincoln, Alliance and Dickens). Our overall strategy was to use RSM in three steps. First, using the method of steepest ascent, we identified the region of CERES-Wheat input variables that gave near maximum yield. Second, we ran a final set of CERES-Wheat simulations to more carefully estimate the surface in the area of the maximum yield and to estimate the optimal inputs  $(X_i)$ . Finally, we evaluated the shape and orientation of the response surface to determine if the optimal  $X_i$ s gave a maximum or saddle point, and to identify a further path of steepest ascent if needed.

CERES-Wheat simulates yield, growth and development of a wheat crop as a function of weather variables, soil characteristics, management practices, and genetic coefficients, which are the coefficients to be used as input variables in CERES-Wheat to represent a particular cultivar (Tsuji et al., 1994). The model uses seven genetic coefficients related to anthesis date, maturity date, grain  $m^{-2}$ , grain weight and grains per spike. Soil characteristics and management factors related to sowing, fertilization and irrigation are also required as input variables. While the model also simulates daily growth and development of the crop based on local weather, we did not use the growth and development variables in subsequent analyses.

In the optimization procedure, five genetic and one management factors were considered as input variables and all other factors were considered fixed. The five genetic factors used as variables were: P1D – the relative amount that development is slowed when plants are grown in a photoperiod 1 h shorter than the optimum (which is considered to be 20 h); P5 – the relative grain-filling duration based on thermal time units (degree-days above a base temperature of 1 °C), where each unit increase above 0 adds 20 degree days to an initial value of 430 degree days; G1 – the kernel number per unit weight of stem (less leaf blades and sheaths) plus spike at anthesis (1/g); G2 – the kernel filling rate under optimum conditions (mg dy<sup>-1</sup> kernel<sup>-1</sup>); G3 – nonstressed dry weight of a single stem (excluding leaf blades and sheaths) and spike (grain ear) when elongation ceases (g). One genetic factor was held constant: P1V, defined as "relative amount that development is slowed for each day of unfulfilled vernalization, assuming that 50 days of vernalization is sufficient for all cultivars" was fixed at six (6) to represent winter wheat.

In this study, Karl 92 was used as a starting cultivar. Karl 92 is adapted to southeastern Nebraska (represented by Lincoln), less so to Dickens, and poorly adapted to Alliance. Genetic coefficients of Karl 92 used in this study were calculated using the GenCalc program in DSSAT v. 3.0 from experimental field data. Plant population density (plants m<sup>-2</sup>), a management input, was varied to find the optimal plant population that maximized yield. Sowing dates used with normal CO<sub>2</sub> were based on current management practices at each site. Sowing dates used with high CO<sub>2</sub> scenarios were chosen to approximate the dates when mean air temperature from high CO<sub>2</sub> scenarios was the same as the mean air temperature of current sowing dates (Table 1). Thus, we assumed no change in germination traits for future cultivars. Nitrogen was held constant at 50 kg/ha, a typical minimum input for wheat in Nebraska. The simulation was run assuming rain-fed production (without irrigation). Current data

Table 1

Sowing dates used for current (normal  $CO_2$ ) and future (high  $CO_2$ ) climatic scenarios at three Nebraska locations

Scenario	Alliance	Dickens	Lincoln
Current (CO <sub>2</sub> = 360 $\mu$ mol/mol)	8 September	18 September	26 September
Future (CO <sub>2</sub> = 720 $\mu$ mol/mol)	29 September	9 October	17 October

Table 2
Predefined ranges for the values of genetic input variables used in the CERES-Wheat model (Tsuji et al.
1994)

Input	Lower limit	Upper limit
Photoperiod sensitivity (P1D)	1.0	4.7
Grain filling duration (P5)	1.0	5.0
Kernel number per spike parameter (G1)	1.1	5.5
Kernel filling rate (G2)	1.3	6.8
Kernel weight parameter (G3)	1.0	4.4

for soil characteristics for each of three locations were also used (Weiss et al., 2003; Won, 2001). It was assumed that the wheat was sown in fallow soil. Initial soil moisture conditions at each site were obtained by running the water balance component of CERES-Wheat 40 days prior to sowing. Other management variables were held constant based on current management practices. It was assumed that no biotic stresses were present while abiotic stresses for temperature, soil water, soil nitrogen and  $CO_2$  concentration were considered. The ranges of the genetic factors were based on the lowest and highest values for the set of winter wheat cultivars listed in DSSAT manuals (Table 2 and Tsuji et al., 1994). The genetic factors were limited to these ranges since the precision of CERES-Wheat predictions beyond these ranges is unknown.

Two different climatic scenarios were used: normal CO<sub>2</sub> (360  $\mu$ mol/mol), based on the mean climate conditions (temperature, solar radiation, and precipitation) of the period 1961–1990, and high CO<sub>2</sub> (720  $\mu$ mol/mol) with future climatic conditions based on the mean conditions of the last 30 years of the 21st century based on HADCM2 (Johns et al., 1997). We used the HADCM2 projections because they were not considered extreme in terms of either over- or underprediction of major climate variables (Southworth, 2002). These projections were used by the National Assessment Synthesis Team (2000) to provide an impact assessment of climate change in the United States. Weiss et al. (2003) also used HADCM2 climate change projections to assess winter wheat responses to climate change scenarios in the winter wheat growing areas in Nebraska.

In order to go from the course grid scale of the Hadley model output to a specific location, the following procedures were used. The historical data for each location, from VEMAP (Kittle et al., 1997) were averaged over 1961–1990 (base data) and the HADCM2 climate change projections data obtained from VEMAP were averaged over 2070–2099. These averages were compared to calculate absolute changes in monthly temperature and solar radiation and relative changes in monthly total precipitation, length of wet and dry periods, and daily temperature standard deviations. The distribution of wet and dry days was not modified, i.e., these distributions were the same as in the original data set. LARS-WG v3.2 (Racsko et al., 1991; Semenov et al., 1998; Semenov and Brooks, 1999) can generate daily values of maximum and minimum air temperature, precipitation and solar radiation from monthly values of these parameters and their associated standard deviations. Once the monthly

absolute and relative changes in the climatic variables and associated standard deviations were determined, actual daily weather data (maximum and minimum temperatures, precipitation, and solar radiation) were used by LARS-WG to generate the climate scenario based on the HADCM2. Different climate scenarios could be generated by changing the mean and standard deviation values of climate parameters. More detail about this weather simulation method can be found in Weiss et al. (2003). One hundred independent stochastically simulated normal and high CO<sub>2</sub> "years" of daily weather data representing the range of average conditions for the last 30 years of each climate scenario were generated for three locations in Nebraska: Lincoln (sub-humid climate; 40°51′N, 96°36′W, 34 m elev.), Alliance (semi-arid climate; 42°30′N, 102°55′W, 1213 m elev.), and Dickens (transition between sub-humid and semi-arid; 40°57′N, 100°58′W, 945 m elev.). These locations are reasonably representative of the major portion of the winter wheat growing areas in the Central Great Plains of the USA (Peterson, 1992).

We ran the CERES-Wheat model using one hundred simulated years' weather under the normal CO<sub>2</sub> concentration and under the doubled CO<sub>2</sub> concentration of 720  $\mu$ mol/mol. RSM was used to identify levels of the six CERES-Wheat input variables that maximized grain yield at the three sites under high CO<sub>2</sub> conditions. A second-order design and model were then used to estimate the response surface near the maximum and finally, canonical analysis was used to characterize the nature of the surface around the maximum.

# 2.1. Finding the area of the maximum: the method of steepest ascent

We used this method to sequentially find an area near the maximum yield using the following steps. The method of steepest ascent allows us to find the values of the six input variables (P1D, P5, G1, G2, G3 and plant density) in the area near the maximum yield.

Step I: Starting values and ranges of experimental factors. Initial starting points for the six input variables were established by using the genetic coefficients for a winter wheat cultivar Karl-92 (Weiss et al., 2003; Xue, 2000) and using the plant population density commonly used by farmers at each location (Table 3). The low and high values for the variables were chosen so that they were sufficiently different to ensure a primarily linear response but not large to induce curvature effects.

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Location	P1D	P5	Gl	G2	G3	Plants/m <sup>2</sup>	
Alliance	2.9	1.5	4.0	2.1	2.0	160	
Dickens	2.9	1.5	4.0	2.1	2.0	200	
Lincoln	2.9	1.5	4.0	2.1	2.0	260	
Range	±0.2	±0.2	±0.2	±0.2	±0.2	±10	

Table 3

Initial values and ranges for CERES-Wheat input variables used in the steepest ascent procedure to identify an area near maximum yield

P1D = photoperiod sensitivity; P5=grain filling duration, G1 = kernel number per spike parameter; G2 = kernel filling rate; G3 = kernel weight parameter (Tsuji et al., 1994).

Step II: First order experiments. In the two input illustration depicted in Fig. 1, the first order experiments around points a and c were  $2^2$  full factorials (i.e., four points around point a and c). Six input variables were considered in this study and use of a full factorial design with two levels for each input factor would require an excessive number of simulations since it would be necessary to run  $2^6 = 64$  design points with 100 years of simulations for each design point (i.e., 6400 simulations). Since the path of steepest ascent is computed from a planar-type of surface obtained by fitting a first-order main effects model excluding interactions, it is only necessary to use a portion of the  $2^6$  design points. In our study, a Plackett–Burman design (PBD) was used because it allows one to evaluate up to n - 1 factors in n design points when n is divisible by four (Lin and Draper, 1992). The first six columns from a PBD with n = 12 were considered to identify the 12 design points for each first-order experiment conducted when using the steepest ascent procedure (Table 4).

Step III: First-order model and the path of steepest ascent. For a given first-order experiment, mean yields over 100 years of simulations were obtained for each of the design points. For example, in Fig. 1 mean yields would be obtained for each of the four design points around point a for the initial experiment or point c for the second first order experiment. Using the mean yields as the values of the dependent variable, the following first-order model was fitted

$$\hat{y} = b_0 + \sum b_i X_i, \quad i = 1, 2, \dots 6,$$

where the slope coefficients  $(b_i)$  were estimated using least-squares and the  $X_i$  were in coded form with  $X_i = +1$  for the high level of the factor and  $X_i = -1$  for the low level. To identify the path of steepest ascent, the largest  $|b_i|$  was identified and the ratio  $b_j/\max|b_i|$ ,  $i \neq j = 1, ..., 6$  was obtained for each variable. Step sizes of  $\Delta X_i = 0.4$  were used and values of  $X_j = \text{ratio } \Delta X_i + \text{ starting value, for each variable were identified as points on the path of steepest ascent. These points were translated to the original$ 

Table 4

Design points for initial first-order experiment at Alliance, NE for CERES-Wheat input variables used in the steepest ascent procedure to identify an area near maximum yield

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Design point	P1D	P5	G1	G2	G3	Plants/m <sup>2</sup>
1	3.1	1.3	4.2	1.9	1.8	150
2	3.1	1.7	3.8	2.3	1.8	150
3	2.7	1.7	4.2	1.9	2.2	150
4	3.1	1.3	4.2	2.3	1.8	170
5	3.1	1.7	3.8	2.3	2.2	150
6	3.1	1.7	4.2	1.9	2.2	170
7	2.7	1.7	4.2	2.3	1.8	170
8	2.7	1.3	4.2	2.3	2.2	150
9	2.7	1.3	3.8	2.3	2.2	170
10	3.1	1.3	3.8	1.9	2.2	170
11	2.7	1.7	3.8	1.9	1.8	170
12	2.7	1.3	3.8	1.9	1.8	150

P1D = photoperiod sensitivity; P5 = grain filling duration, G1 = kernel number per spike parameter; G2 = kernel filling rate; G3 = kernel weightparameter (Tsuji et al., 1994).

scales for the six CERES-Wheat input variables and the CERES-Wheat was run for each of the points on the path. Simulations were run for points along the path until either the mean of the simulated yield was substantially less than the predictions from the first-order model or until the mean yield decreased substantially. We also stopped making runs on the path if at least one of the genetic values exceeded the range predefined in Table 2. In either case, we stopped, returned to step II, another PBD was set up at that point and continued. If any genetic input was out of range, the value for that input was fixed as predefined and additional first-order experiments were conducted varying the remaining inputs.

Step IV: Terminating steepest ascent. The steps II to III were repeated until either (1) all the least-squares slope coefficients  $(b_i)$  were small or (2) only a small increase in yield was obtained by additional runs on the path, or (3) the harvest index achieved a value of 0.5, the highest achievable value (Slafer et al., 1999).

2.2. Simulation experiments near the area of the maximum: Second order design and model

Assuming the method of steepest ascent identifies the values of the CERES-Wheat input variables near the maximum yield, an appropriate experimental design and estimated response surface are then needed to precisely estimate the input values that maximize yield. A central composite design (CCD) was used to identify the design points for the final set of simulation runs (Myers and Montgomery, 1995). Using the means of the simulated yields for the points from the CCD, the following second order model was fitted

$$y_{ij} = b_0 + \sum b_i X_i + \sum b_{ii} X_i^2 + \sum \sum b_{ij} X_i X_j, \quad i, j = 1, \dots, k,$$

where bs are the linear  $(b_i)$ , quadratic  $(b_{ii})$  and cross-product  $(b_{ij})$  regression coefficients estimated using least-squares and k is the number of input variables in the final experiment. In matrix notation, the model is written as

$$y = b_0 + X'b + X'\mathbf{B}X,$$

where  $X' = \text{row vector of input values} = [X_1X_2...X_k]; b' = [b_1b_2...b_k]$  a row vector of linear slope coefficients, **B** = a matrix of quadratic and cross-product regression coefficients. These b coefficients were estimated using least-squares and the fit of the model was evaluated using  $R^2$ . The significance of each model term (linear, quadratic and cross product) was tested using residual error variance.

#### 2.3. Identifying input levels that maximized yield and evaluation of the surface

Values of the experimental variables that maximized yield were determined by differentiating the second order model, equating the derivative to zero and solving for X. More specifically,  $\partial y/\partial X = b + 2\mathbf{B} X = 0$  which implies that  $X_0 = -1/2 \cdot \mathbf{B}^{-1} \cdot b$ , where  $X_0$  is the stationary point and the value of yield at the stationary point is  $y_0 = b_0 + X'_0 \mathbf{B} + X'_0 \mathbf{B} X_0$ , where  $\mathbf{B}^{-1}$  is the inverse of  $\mathbf{B}$ . To evaluate the surface in the area of the optimum, the second order model was transformed to the canonical model,

$$y = y_0 + \sum \lambda_i W_i^2,$$

where the  $\lambda_i$  are eigenvalues of **B** and the  $W_i$  are the canonical variables (Myers and Montgomery, 1995). The  $W_i$  are the variables for transformed axes that identify the orientation of the second-order response surface. The canonical model is useful (1) for determining if the stationary point is a maximum, minimum or saddle point and (2) to evaluate the change in yield as one moves from the stationary point to nearby points. The  $\lambda_i$  values identify the nature of the stationary point. If the  $\lambda_i$ are all negative then any movement away from the stationary point will reduce y and so  $X_0$  is a maximum. Similarly, if all the  $\lambda_i$  are positive,  $X_0$  is a minimum and when the  $\lambda_i$  are mixed signs  $X_0$  is a saddle point.

The estimated surface was characterized on the basis of the following criteria: Case I: If the stationary point determined by the model was inside the experimental region and all  $\lambda_i$  were less than zero, the stationary point,  $X_0$  was the point of maximum yield response. Case II: If the stationary point was outside the range of the second-order design points and some  $\lambda_i$  were less than zero and some were greater than zero, the stationary point,  $X_0$  was a saddle point. The saddle point can be evaluated by values of  $-\lambda_i$  and  $+\lambda_i$ . When the response surface was a saddle, a ridge of steepest ascent was estimated and further simulation runs on these ridges were conducted until there was only a slight increase in yield and this final point was considered maximum.

## 3. Results and discussion

The Hadley (HADCM2) based scenario projected a mean annual monthly temperature greater (3 °C) than the observed data over the calendar year. A similar temperature increase was obtained under the HADCM2 scenario during the winter wheat growing season (September–June). During the calendar year, the mean total monthly precipitation increased under the HADCM2 based scenario with a 17% (~5 mm), 21% (~12 mm), and 25% (~15 mm) for Alliance, Dickens, and Lincoln, respectively. During the winter wheat growing season, the scenario projected 21% (~6 mm), 26% (~14 mm), 26% (~14 mm) increases in monthly precipitation at Alliance, Dickens, and Lincoln, respectively. Similarly, the mean annual monthly solar radiation from the HADCM2 scenario projected decreases of 0.84, 0.98, and 0.94 MJ m<sup>-2</sup> d<sup>-1</sup> for Alliance, Dickens, and Lincoln, over the calendar year. During the growing season, decreases in solar radiation of 0.81, 0.96 and 0.89 MJ m<sup>-2</sup> d<sup>-1</sup> at Alliance, Dickens, and Havelock were observed under the HADCM2 scenario.

Once the surface was obtained in the area of the optimum from the second order model, further simulation runs on the ridge of steepest ascent were conducted to check the sensitivity of the simulated yield. In all cases, only slight changes in yield were observed around the optimum. It is also important to note that the optimum points identified in this study were within the ranges of the genetic coefficients for all the winter wheat cultivars given in the DSSAT manual and had a harvest index of no more than 0.5. To evaluate the validity of this approach (the path of steepest ascent), an optimal cultivar was obtained based on the characteristics of Karl 92 for 100 years of simulated weather data for the normal  $CO_2$  conditions. These simulated weather data, generated using LARS-WG, had the same statistical distributions as the current weather data for Alliance, NE. The resulting simulated yield was 3447 kg/ha (data not shown here). The mean value of the observed yields for the four highest yielding cultivars over the last five years at Alliance, NE was 2753 kg/ha, on a dry weight basis. CERES-Wheat does not deal with abiotic (except for high temperatures and water stress) or biotic stresses nor does it deal with harvest losses. Thus this difference, about 25% relative to the simulated value, is quite reasonable when taking into account the assumptions found in CERES-Wheat and the realities of the observed values.

The optimum values obtained for the genetic factors indicated that the optimal cultivar for the future high  $CO_2$  conditions should have less photoperiod sensitivity (P1D), long grain filling duration (P5) and a high kernel filling rate (G2) (Table 6). These results agreed with Hall and Allen (1993) who found that cultivars for future climatic conditions should extend the grain filling period, shorten the duration of vegetative growth (which would also improve harvest index) and be adapted to photoperiod. Our results also agreed with Lawlor and Mitchell (2000) and Rawson and Richards (1992) who claimed that control of photoperiod and vernalization sensitivity would be necessary for future climatic conditions.

For each location, agronomic results are presented for three cases: Karl 92, under normal  $CO_2$  conditions, Karl 92 under high  $CO_2$  conditions and the new cultivars determined by RSM under high  $CO_2$  conditions (Table 5). The effect of elevated  $CO_2$  on Karl 92 was not observed in this study, which may have been due to the negative effect of warmer temperatures and changes in precipitation pattern. Mitchell et al. (1995) and Wheeler et al. (1996) found that the increased temperature reduced harvest index and grain yield proportionately. However, within the optimum temperature range, the beneficial effects of  $CO_2$  enrichment may be sufficient to counterbalance the negative effects of rising temperature if other factors are not limiting.

In all three cases, increasing trends of yield were observed from semi-arid (Alliance, NE), transitional (Dickens, NE) to subhumid (Lincoln, NE) environments (Tables 5). Overall, the results indicated that the 'optimal' cultivar under high CO<sub>2</sub> conditions produced 1.65–2.5 times more yield than Karl 92 under normal CO<sub>2</sub> conditions (Fig. 2 for Alliance, other two locations are not shown). This study also revealed that the optimal cultivar had 1.2–1.35 times more kernel weight and 1.35–1.9 times more kernels m<sup>-2</sup> than Karl 92 under normal CO<sub>2</sub> conditions (Fig. 2). In addition, the optimal plant density under high CO<sub>2</sub> conditions was from 1% to 19% less than the currently used plant densities. At all locations, the optimal cultivars under high CO<sub>2</sub> had shorter days to flower, grew faster, and had more grain m<sup>-2</sup> than Karl 92 under normal CO<sub>2</sub> conditions, and yield was improved under high CO<sub>2</sub> conditions by sowing three weeks later than normally practiced (Table 5). Table 5

Variable	Lincoln			Dickens			Alliance		
	Karl92-360	Karl92-720	New-720	Karl92-360	Karl92-720	New-720	Karl92- 360	Karl92-720	New-720
Seeding date	26 September	17 October	17 October	18 September	09 October	09 October	08 September	29 September	29 September
Plant population (m <sup>-2</sup> )	260	260	238	200	200	198	160	160	132
Flowering date	26 May	18 May	19 May	1 June	21 May	18 May	05 June	23 May	13 May
Physiological maturity	25 June	17 June	21 June	4 July	21 June	19 June	07 July	24 June	17 June
Grain yield (kg/ha)	3370	3370	5810	2870	3100	5110	1990	2610	5090
Weight/grain (mg)	30.4	30.1	37.2	30.1	29.3	37.78	28.3	28.9	38.1
Grains $(m^{-2})$	11,100	11,200	15,600	9500	10,600	13,500	7000	9000	13,300
Leaf area index $(m^2/m^2)$	3.37	3.18	2.96	2.48	2.73	2.64	2.34	2.89	2.64
Biomass at anthesis (kg/ha)	6660	6120	6560	5150	5290	5280	4920	5170	5320
Biomass at harvest (kg/ha)	10,300	10,200	11,600	8300	9300	10,000	6900	8300	9900
Stalk at harvest (kg/ha)	6900	6820	5770	5470	6230	4880	4890	5730	4780
Harvest index (kg/kg)	0.33	0.33	0.5	0.34	0.33	0.5	0.28	0.31	0.50

Wheat plant and required management for maximum yield at Lincoln, Dickens and Alliance, NE under high  $CO_2$  and current climatic conditions (Karl92 = 'Karl 92'; New = 'optimal cultivar'; 360 = 'normal  $CO_2$  conditions'; 720 = 'high  $CO_2$  conditions')

Factors	Karl92	New_720						
		Alliance	Dickens	Lincoln				
P1V	6	6	6	6				
P1D	2.9	1	2.3	1.9				
P5	1.5	2	1.6	4.7				
G1	4	5.5	5.2	5.5				
G2	2.1	4.8	3.5	6				
G3	2	2	2	2				

Genetic coefficients for Karl 92 and new varieties for each location (New = 'optimal cultivar'; 720 = 'high CO<sub>2</sub> conditions')

P1D = photoperiod sensitivity; P5 = grain filling duration, G1 = kernel number per spike parameter; G2 = kernel filling rate; G3 = kernel weight parameter (Tsuji et al., 1994).



Fig. 2. Grain and biomass components, as proportion of Karl 92 under normal conditions at Alliance, NE for four cases: Karl92; New = 'optimal cultivar'; 360 = 'normal CO<sub>2</sub> conditions'; 720 = 'high CO<sub>2</sub> conditions'.

The optimum values for the genetic factors of the best future cultivar make biological sense. The lower photoperiod response clearly will be needed since the predicted future warmer temperatures will delay sowing and make flowering earlier. Wheat is generally planted after the Hessian fly (*Mayetiola destructor* Say) free date, which is based upon the average, first fall freeze. With predicted warmer temperatures, the freeze will occur later and the sowing should also be later. Cultivars with a lower photoperiod requirement are needed to avoid warmer temperatures during the current grain filling period. Cultivars with a greater (longer day) photoperiod response would delay flowering until the warmer part of the growing season, which would reduce potential grain yields. Historically, cultivars developed in Nebraska are more photoperiod sensitive than cultivars developed in the southern Great Plains. Presumably the photoperiod requirement was to avoid late spring freezes that damage early flowering cultivars. With warmer temperatures, delayed flowering would no longer be needed to avoid spring freezes. As expected, predicted earlier flowering led to earlier maturity.

Table 6

In this study, we used Karl 92 for our model cultivar. Karl 92 is adapted to southeastern Nebraska (represented by Lincoln), less so to Dickens, and poorly adapted to Alliance (as evidenced by the reduced grain yield at Dickens and Alliance when compared to Lincoln). Hence it was not surprising to see the greatest grain yield difference between Karl 92 and the new cultivar at Alliance. One surprising result was the predicted earlier physiological maturity at Alliance for the new cultivar at 720  $\mu$ mol/ mol CO<sub>2</sub> than at Dickens and Lincoln. Presumably this result was due to the drier climate at Alliance than at the other two sites.

While these predictions are rough approximations, they do provide insights to future wheat cultivars and cropping practices. For example, hard winter wheat is usually milled to produce bread flour. The protein requirements for such flour are 12%(120 mg of protein per 1 g of flour). To increase grain yield by 65-150% while retaining the protein content will require a greatly increased use of nitrogen fertilizers that will have to be applied in an ecologically sound manner. Cultural practices that reduce water loss from the soil will be important in these new cropping systems. Similarly, the increased straw production per hectare will require careful management. Finally, the cropping system may need to change to reflect the greater time available for a rotational crop. For example at Alliance, the new cultivar at 720 µmol/mol will be planted 21 days later and harvested 20 days earlier than wheat is today. Hence up to an extra 41 days would be added to the summer growing season, which may increase the choices for rotational crops.

In this study, application of this methodology to winter wheat in the USA Great Plains tended to support the conclusion that under high  $CO_2$  – high temperature conditions, translocating more energy to produce more and heavier kernels and less energy to the vegetative parts of the plant could result in dramatically higher yields without substantially changing crop management practices except planting dates. This type of information can be only considered preliminary since it is strongly based on the assumptions that the weather and plant simulation models produce good predictions. For example, CERES-Wheat responds to mean temperature, while crops actually develop under sinusoidal day-night temperature of varying amplitude. Regardless of this limitation, the approach can be a valuable tool in assessing how climate changes may impact winter wheat production in the US Great Plains and the type of germplasm that plant breeders will need to develop in the years to come.

Identifying appropriate agronomic technologies that may be needed for future climatic conditions is difficult since (1) it is quite difficult to conduct field experiment to approximate the long term selection process under future climatic conditions and (2) experiments that approximate future climate conditions are by necessity quite small, and can not be used to evaluate a large number of cultivars and/ or agronomic practices that would be needed in order to identify the optimal configuration of plant traits and agronomic practices. Using response surface methodology in conjunction with crop and weather simulation models may allow researchers to identify combinations of plant traits and management practices that indicate needed changes in managed field crop systems as a result of future climate scenarios. The approach can be useful in understanding the complex relationships among crop genotypes, climate and management, for comparing various crop and weather models regarding the theoretical optima and can be a useful tool to agricultural scientists and policy makers who are assessing how climate change may impact the agriculture and society.

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