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Simulating Crop Phenological Responses to Water Stress using the PhenologyMMS Software Component

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Abstract: Crop phenology is fundamental for understanding crop growth and development, and increasingly influences many agricultural management practices. Water deficits are one environmental factor that can influence crop phenology through shortening or lengthening the developmental phase, yet phenological responses to water deficits have rarely been quantified. This paper describes the development and statistical evaluation of the PhenologyMMS V1.2 software component for simulating the phenology of various crops at different levels of soil water content. The component is intended to be simple to use, requires minimal information for calibration, and can be easily incorporated into other crop simulation models. PhenologyMMS evaluation consisted of utilizing data from a variety of field experiments to test algorithms for different crops (using "generic" phenology parameters with no calibration for specific cultivars) to predict developmental events such as seedling emergence and physiological maturity. Results demonstrated that the PhenologyMMS component has general applicability for predicting crop phenology and has the potential, if coupled to mechanistic cropping system models (e.g., DSSAT and APSIM), to improve model ability to simulate phenological responses to environmental factors.

***Keywords**:* Component-based modeling; Phenology; Crop development; Growth stages; Model reusability.

1. INTRODUCTION

One of the factors limiting the development of environmental (e.g., agricultural, biophysical, and ecological) models in general has been the inability of any single group of researchers to deal with the conceptual complexity of formulating, building, calibrating, and debugging complex models. The need for collaborative model building has been recognized for at least 20 years in the environmental sciences [Acock and Reynolds 1990; Reynolds and Acock 1997]. Model development architecture (i.e., concepts and methodology) based on reusable components was presented by Papajorgji et al. [2004] and Rizzoli et al. [2008] among others for agro-environmental models and by Castronova and Goodall [2010] among others for hydrologic models. Although component-based software engineering techniques have long been recommended by the crop modeling community [Jones et al. 2001] with subsequent adoption in the DSSAT v4.5 and APSIM model development efforts [Keating et al. 2003], in general crop model developers have not embraced component-oriented model design in a systematic or coordinated fashion. A component-based approach for cropping system simulation is desirable for several reasons including: 1) it should help model developers add new components to include new algorithms with minimal changes to existing code, and 2) it should allow model developers to update documentation and to maintain code much more effectively. One goal of a modular approach is to allow scientists in different disciplines to develop modules using their knowledge, data, and expertise and not be burdened with development and maintenance of code for other components [Jones et al. 2001].

Acock and Reynolds [1989] and Reynolds and Acock [1997] also proposed criteria for a generic modular structure for crop models. A process within the crop discipline that naturally lends itself to a modular modeling structure is phenology, i.e., the sequence and timing of developmental events or stages and the interaction with climate. Phenology is fundamental in understanding crop development and growth. Farmers increasingly are basing management on crop phenological events to enhance economic crop yields while maintaining environmental quality. One deficiency in accurately predicting phenology in variable environments and management systems is that little research has examined the impacts of water deficits (degree, timing, and history) on crop phenology [McMaster et al. 2009], despite the obvious influence of water deficits on some developmental phases (e.g., seedling emergence, grain filling duration). Further, phenological responses to water deficits vary among crops, cultivars, and developmental events. With few exceptions, crop phenology simulation models do not consider the influence of water deficits on phenology. Without quantification of phenological responses to water deficits for specific crops, a suitable foundation does not exist to predict crop development under variable environmental conditions. Such a foundation to transfer knowledge, presented in the form of a self-contained, reusable software component, would aid in developing decision support technologies and improve crop model ability to simulate phenological responses to environmental factors such as limited soil water.

Previously, McMaster et al. [2011] provided an overview of PhenologyMMS V1.2 (Modular Modeling Software) with a focus on the Java-based interface. The objectives of this paper are to: 1) describe the development and evaluation of the PhenologyMMS V1.2 component for simulating the phenology of various crops at different levels of soil water; and 2) determine whether the scientific approach used in PhenologyMMS improved the accuracy of phenological predictions by incorporating the influence of water deficits. The basic science behind the component is described, and general output responses/statistical evaluation of the component for simulating phenology are presented.

2. MATERIALS AND METHODS

2.1 PhenologyMMS component description

The PhenologyMMS component was designed, with guidelines proposed by Jones et al. [2001] in mind, as an autonomous FORTRAN module requiring input data for plant parameters, daily weather data, and initial conditions. For several reasons, including making the component easier to access and facilitating the use and evaluation of the component, a simple Java-based interface was developed [McMaster et al. 2011]. Inputs required by the PhenologyMMS component are weather data, general agronomic management information, and plant parameters. Required weather data are daily maximum and minimum air temperature (^{o}C) and precipitation (mm; only needed for the time period from planting to emergence). Basic agronomic information related to initial conditions is required including planting date, depth, and rate; the phyllochron (i.e., the rate of leaf appearance per unit growing degree-day); final canopy height; and latitude of the location. Default values are provided for each crop and set for northeastern Colorado USA, and can be changed as desired by the user. Other required plant parameters, with default values for each crop, include cardinal temperatures used in calculating thermal time; germination and elongation rate values for different levels of soil moisture at planting; and phenological thermal time values for each developmental phase simulated that are adjusted for water deficit levels and by either cultivar or maturity class.

The initial science behind the approach for simulating crop phenology in the Phenology MMS component was based on an earlier and more detailed phenology model for wheat and barley [SHOOTGRO, McMaster et al. 1992]. In

PhenologyMMS, the user can choose between two extreme levels of water deficits (see Figure 1). The *No Stress* option refers to non-limiting conditions of soil water availability (e.g., field capacity). This option should be selected for irrigated or high rainfall conditions. The *Stressed* option refers to the most limiting value of water deficits not leading to terminal stress (i.e., just above permanent wilting point). This option should be selected for most rain fed situations where soil water may be severely limiting. Because conditions are often between the *No Stress* and *Stressed* extremes, the user can either estimate which option is closest to the conditions to be simulated and select that option, or change the default values to an intermediate option between the two extremes.

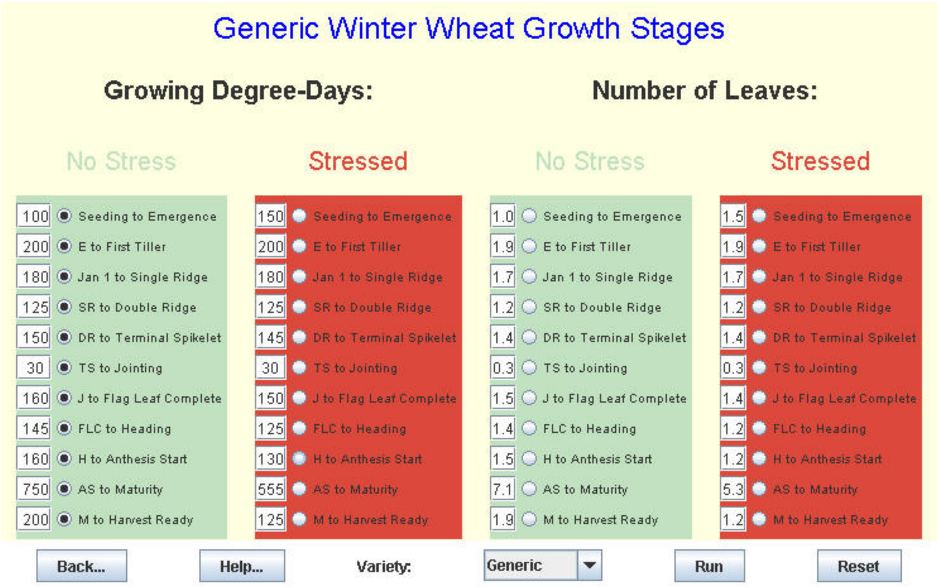

Figure 1. Set Growth Stages screen in PhenologyMMS. The default parameters for developmental stages (under *No Stress* and *Stressed* conditions) for a generic winter wheat plant are shown. (From McMaster et al. 2011)

Two additional sub-components are included in the PhenologyMMS component: a seedling emergence component and canopy height component. When the PhenologyMMS component is run using the interface driver, an output file is automatically generated which contains all initial conditions and parameter values used in the run. The output file includes a table with the simulation dates and thermal time from planting, emergence, and fully vernalized (if appropriate) for each developmental event. Leaf number over time and final canopy height are also given.

2.2 Data sets and model evaluation criteria

Evaluating the PhenologyMMS component required collecting data sets (for both model development and evaluation) for the following crops: 1) winter and spring wheat (*Triticum aestivum* L.); 2) corn (*Zea mays* L.); 3) sorghum (*Sorghum bicolor* L.); 4) proso millet (*Panicum milaceum* L.); 5) hay/foxtail millet [*Setaria italica* (L.) P. Beauv.]; and 6) sunflower (*Helianthus annus* L.). The data sets were used to evaluate PhenologyMMS crop development and leaf production predictions and were derived from multiple cropping system experiments across the U.S. Central Great Plains. Each data set varied on methodology for measuring phenology, which developmental events were measured, and the environmental and management factors included. Studies typically included multiple cultivars for each crop and both irrigated and dryland (non-irrigated) conditions. Water deficit levels were not rigorously measured in all studies; nevertheless, the data sets are useful in providing a general evaluation of the reasonableness of the PhenologyMMS component in simulating developmental events using the default parameters for each crop. While the phenology data measured differed depending on crop, in general major developmental stages (e.g., seedling emergence, beginning of stem elongation, flag leaf blade growth complete, anthesis, and physiological maturity) were measured from one to three days per week.

The most conservative evaluation approach was used for winter and spring wheat where the default parameters for a generic cultivar from a crop were used in all simulations. This was preferred because the data sets were so extensive in terms of cultivars, treatments, environmental conditions, and management practices that this would provide a good evaluation for users that have little information. Similarly, the conservative approach was chosen for proso millet, hay millet, and sunflower because we lacked developmental knowledge of the cultivars. For sorghum and corn we had more cultivar developmental knowledge and selected the general maturity classes (e.g., early maturity, medium maturity, late maturity for sorghum, and maturity groups such as 105-day, 110-day, etc. for corn). For all simulations, soil water was set to "optimum" at planting, default planting depths were used (Table 1), and the default values for the *Stress*ed option selected unless the data were for an irrigated treatment.

Table 1. Germination and seedling elongation rate parameters for specific crops and seedbed conditions.

Soil Moisture	Winter Wheat	Spring Wheat	Corn	Sunflower	Sorghum	Proso Millet	Hay Millet
Germination (∑GDD[a]):							
Optimum[b]	80.0	80.0	7.5	40.0	40.0	80.0	80.0
Medium	90.0	90.0	10.0	50.0	50.0	90.0	90.0
Dry	110.0	110.0	20.0	70.0	70.0	110.0	110.0
Dust[c]	700.0	700.0	500.0	500.0	500.0	700.0	700.0
Elongation rate (mm/GDD):							
Optimum	0.50	0.50	2.5	1.5	1.5	0.50	0.50
Medium	0.40	0.40	1.75	1.0	1.0	0.40	0.40
Dry	0.33	0.33	1.5	0.6	0.6	0.33	0.33
Dust	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Planting depth (cm):	5	4	4.5	5	5	2	2

[a] Accumulated growing degree-days (GDD) required to initiate germination.
[b] Seedbed conditions are based on % water-filled pore space: optimum (>45%), medium (35-45%), dry (25-35%), and dust (<25%).
[c] Soil moisture in this category is below the minimum threshold to initiate imbibition processes.

Relative error (RE) and Root Mean Square Error (RMSE) evaluation statistics were calculated to compare modeled results to measured data. Relative error was expressed in percent as:

$$RE = \frac{\left(\overline{P} - \overline{O}\right)}{\overline{O}} * 100 \qquad (1)$$

where $\overline{P}$ is the predicted mean and $\overline{O}$ is the observed mean. The RMSE was calculated by:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} \left(P_i - O_i\right)^2}{n}} \qquad (2)$$

where P_i is the ith predicted value, O_i is the ith observed value, and n is the number of data pairs.

3. RESULTS AND DISCUSSION

In this paper, PhenologyMMS component evaluation primarily focuses on the seedling emergence and physiological maturity developmental events even though many other developmental events were evaluated (data not shown). In evaluating the seedling emergence sub-model, initial soil water in the seedbed at planting was always set to optimum conditions and the default planting depth was used (Table 1). A simulation bias of predicting seedling emergence too early, particularly for corn, proso millet, and sunflower, is shown in Figure 2. This was expected as initial soil water conditions often deviated from optimum conditions or with shallower planting depths. Depending on the crop, the RMSE for seedling emergence ranged from 1.8 days (sorghum) to 9.0 days (corn) and the bias also varied among crops (Figure 2). The extremely accurate and unbiased (RE = 0.20%) simulation of sorghum seedling emergence was encouraging, yet this may mask overestimates of parameters for germination, elongation rates, and planting depths (Table 1) if seedbed soil water was not “close” to optimum (unknown). Conversely, earlier simulated corn seedling emergence (RE = -5.82%) may indicate that actual soil water conditions were less than optimal or planting depths were deeper than default values.

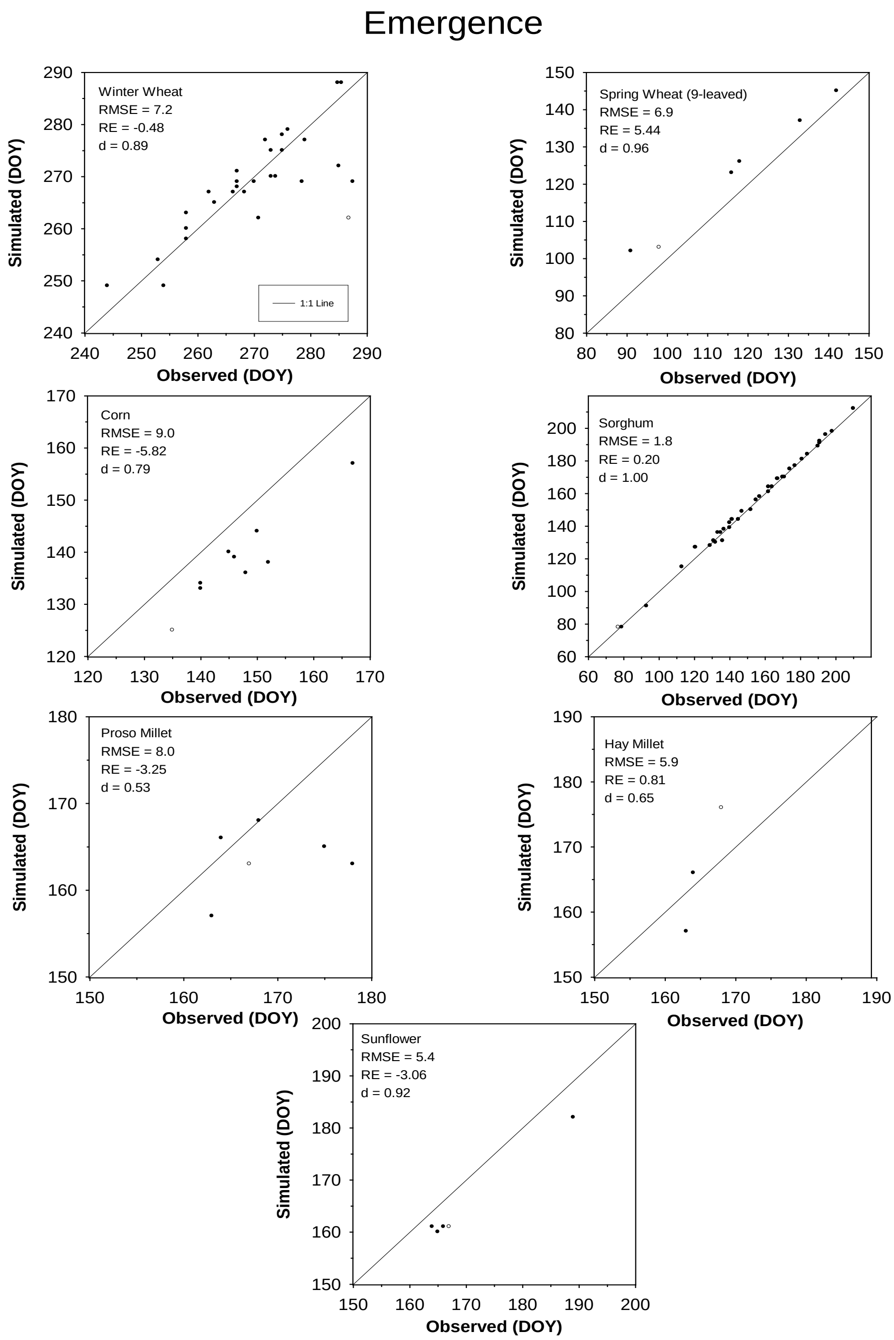

Figure 2. Phenology MMS seedling emergence predictions for various crops.

With the exception of winter wheat and proso millet, where simulated seedling emergence occasionally occurred too early for the latest dates (i.e., DOY), it appears that the seedling emergence model had no bias based on date (Figure 2). The general simulation results presented here seem acceptable given the lack of formal calibration of the inputs to the component.

The duration of grain filling and time of physiological maturity are significantly influenced by the interaction of temperature and water deficits. Cultivars can vary considerably in their response to these two environmental factors [McMaster and Wilhelm 2003; McMaster et al. 2009]. RMSE increased for most crops for simulating physiological maturity when compared to seedling emergence (Figure 3). One factor influencing this was simulating late-maturity cultivars for sorghum and corn resulted in insufficient thermal time accumulation in the fall so that maturity was occasionally simulated in the spring. Frost also can kill or stop further development of sorghum, thus many late planting dates and late maturity cultivars did not reach maturity in the fall. For late-maturing cultivars, it appears that thermal time estimates for grain filling are too high.

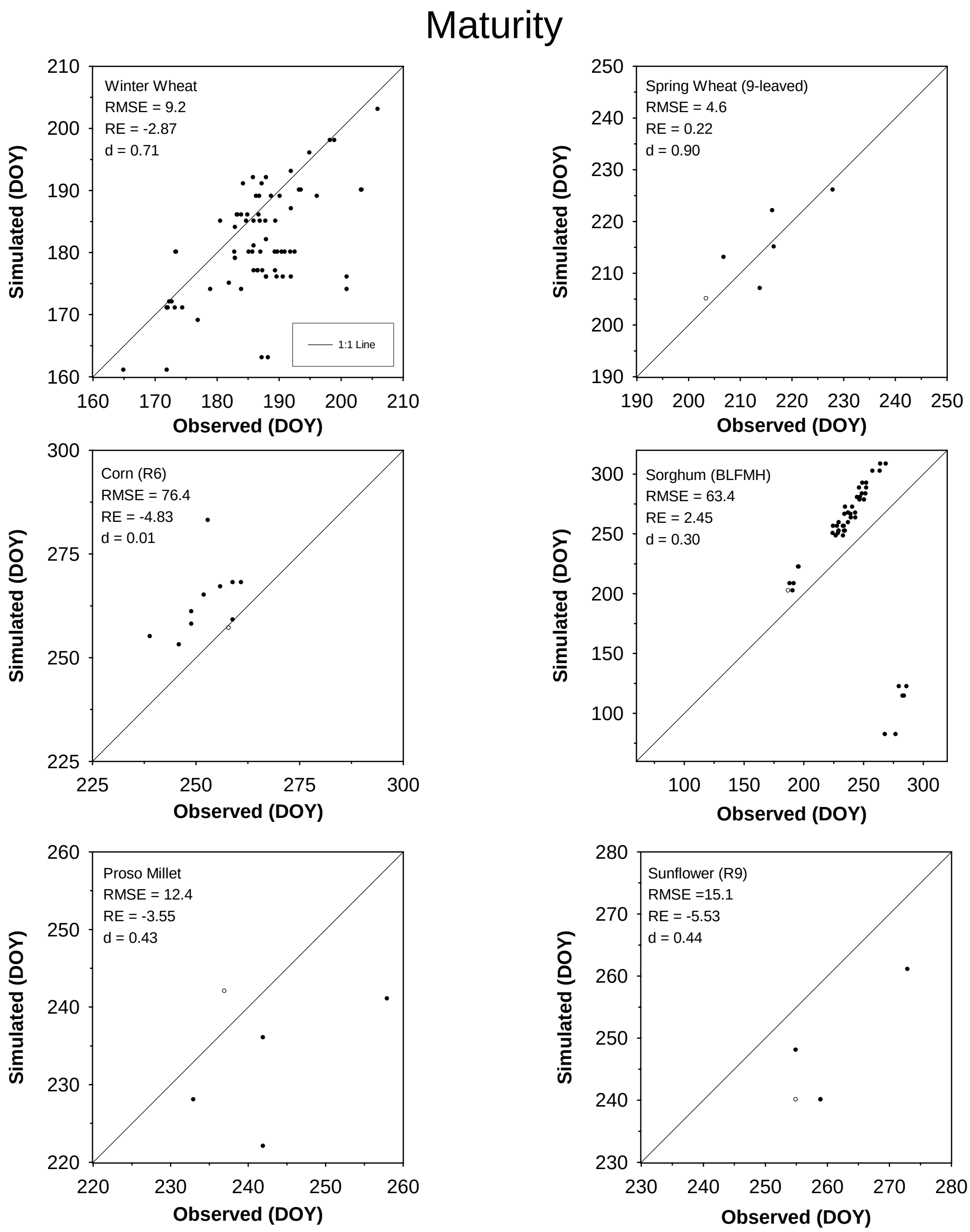

Figure 3. Phenology MMS physiological maturity predictions for various crops.

Table 2. Water deficit model evaluation results using three different default parameter scenarios for sorghum.

Statistics[a]	GN or GS[b]	GN only	GS only
Floral initiation			
RMSE (days)	4.8	4.8	4.8
RE (%)	1.5	1.5	1.5
Flowering/anthesis			
RMSE (days)	18.5	16.3	19.0
RE (%)	8.0	6.9	8.5
Physiological maturity			
RMSE (days)	63.4	63.5	60.4
RE (%)	2.5	3.2	1.8

[a] Model evaluation statistics are root mean square error (RMSE) and relative error (RE).

[b] GN: irrigated/high precipitation soil water level; GS: dryland/low precipitation soil water level.

One important hypothesis of this study was whether the scientific approach used in the PhenologyMMS component improved the accuracy of phenological predictions by incorporating the influence of water deficits. To partially answer this question, we selected sorghum because a fairly even balance between dryland and irrigated data sets were available and then ran the PhenologyMMS component using different default parameters (and assumed optimal soil water conditions at planting and default planting depth). Three approaches were used: 1) either the parameters for non-limiting soil water conditions (parameter GN) or limiting soil water conditions (parameter GS) were selected based on whether the site was irrigated or dryland, respectively; 2) the GN parameters were used for all sites (whether dryland or irrigated), and 3) the GS parameters were used for all sites (whether dryland or irrigated). Results of the three sets of runs for three developmental stages are shown in Table 2. As expected, no difference between the three sets of runs was found for the developmental stage of floral initiation due to equal thermal time from emergence to floral initiation for both GN and GS parameters (450 GDD for a medium maturity cultivar). Slight, but contradictory, differences were found among the runs for the developmental stages of anthesis and physiological maturity. For anthesis, using only the GN parameters for all data sets resulted in the most accurate predictions, and using only GS parameters for all data sets resulted in the least accurate predictions. Because the simulated day of anthesis was biased towards being predicted later than the observed day for both irrigated and dryland sites (data not shown), using only the GN parameters (which had less thermal time from floral initiation to anthesis - 480 GDD for medium maturity cultivars) rather than the GS parameters (505 GDD) reduced the bias of the dryland sites and improved model accuracy (data not shown). It should be noted that if the default GN and GS parameters were reduced to eliminate this initial bias, then the most accurate simulation of anthesis would be achieved by using the GN/GS parameters for irrigated and dryland sites. The opposite results were found for maturity where using only the GS parameters for all data sets resulted in the most accurate predictions, and using only GN parameters for all data sets resulted in the least accurate predictions. The reason for these results is the same as for anthesis: thermal time from anthesis to maturity was less for GS (640 GDD for a medium maturity cultivar) than GN (690 GDD) and this reduced the error in predicting the irrigated sites. If the corrections to the default parameters of both GS and GN from floral initiation to anthesis were made, then again the approach used in the PhenologyMMS component would result in the most accurate prediction of maturity. Even if no adjustment is made to the GN or GS parameters, overall the approach using both GN (for irrigated) and GS (for rain fed) parameters was best when predicting multiple developmental stages.

4. SUMMARY AND OUTLOOK

Modeling of environmental systems is challenging in part because process interaction often spans several disciplines, making it difficult to model integrated system response. Widespread utilization of a hierarchical/modular design of process-based simulation components should facilitate reliable and economical model construction. Furthermore, componentization of environmental models should also reduce repetitive code because it allows model developers to share process-level components so that unique (i.e., customized to the problem at hand) environmental models can be created with reusable components [Argent et al. 2006]. PhenologyMMS V1.2 is intended to provide a well-designed software component to understand and predict crop phenology and how phenology responds to varying water deficits. The evaluation results presented here indicate that the PhenologyMMS component, even when using default parameters and having uncertain inputs, correctly responds to varying water deficits and has reasonable accuracy in predicting crop development. Therefore, it can be used in a number of potential applications, e.g., PhenologyMMS was run using historical weather data at ten different sites in the Central Great Plains to estimate the mean and range of dates for different winter wheat developmental events. This provided the predicted timing of developmental events needed for regional management practices based on development stage [McMaster and Wilhelm 2010].

Future model enhancements based on feedback from users (not discussed in this paper) and the evaluation results include: 1) adding and validating more crops; 2) implementing vernalization and photoperiod factor sub-components; and 3) providing more cultivar or maturity class choices. To better address the issue of quantifying phenological responses to varying water deficits, the PhenologyMMS component is being integrated into an existing crop growth model (based on the WEPS plant growth model) that has a water balance sub-model. Finally, further application of PhenologyMMS could be to explore different possible or projected changes in climate using GCM-generated weather data, although particular caution is warranted until photoperiod and vernalization factors are included in the model. The PhenologyMMS V1.2 software may be freely downloaded from http://www.ars.usda.gov/services/software/download.htm?softwareid=238.

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