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Crop simulation models: Where do we go from here? ^{1, 2}

Modelos de simulação de culturas agrícolas: para onde vamos?

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Abstract - The purpose of this paper is to provide some insights about future directions for crop simulation modeling. The paper begins with some early publications in this area as well as some reasons for the limited number of crop simulation models that are in wide spread use. A philosophical overview on how to approach using, modifying existing, or developing new crop simulation models follows. In order to get the "right" answers for the "right" reasons, one should select an appropriate model for the problem and have an understanding of the non-linear, interrelated nature of many of the algorithms that comprise a model. In the development of future crop simulation models, or the modification of existing models, one shouldn't forget important earlier works, which may provide some unique insights. Nor should one neglect current literature, either by a thorough literature review or by reanalyzing published data. While future crop simulation models will still need to simulate leaves, roots, stems, and reproductive organs; the mechanisms by which they simulate organ level responses will be based on a genetic understanding of a specific cultivar. Crop simulation modeling may play an important role in undergraduate education as a capstone course that integrates knowledge about interactions in the soil-plant-atmosphere continuum. Similarly, it could provide the basis for lessons about plant or soil sciences to students in the K-12 grades. This paper concludes with an interpretation of jogo de cintura, the ability to creatively use available resources, as it relates to crop simulation modeling.

Key words: crop simulation, modeling, perspectives, genomies, future directions

Background

Crop simulation modeling has its roots in the works of MONSI and SAEKI (1953), KANASAGI and MONSI (1954), de WIT (1965), MONTEITH (1965), DUNCAN et al. (1967), STEWART and LEMON (1969), and LEMON et al. (1971). An incomplete list (given that a complete list would be very difficult to assemble, also see the quote from Gleick below) of important papers in the development of crop simulation modeling are: CURRY (1971), CURRY and CHEN (1971), HESKETH et al. (1971), BAKER et al. (1972), FICK et al. (1973), SPLINTER (1974), HOLT et al. (1975), ARKIN et al. (1976), THORNLEY (1976), SINCLAIR et al. (1976)

ACOCK et al. (1978), CHARLES-EDWARDS (1978), HUNT and LOOMIS (1979), and MEYER et al. (1979). Current reviews of crop simulation models can be found in HOOGENBOOM (2000) and in volume 18 (numbers 1–4) of the European Journal of Agronomy published in 2002 and 2003. An interesting aside in this history, while not directly in the area of crop simulation modeling, is the paper by HENRYA. WALLACE, WALLACE (1920); Wallace was the founder of Hi-Bred Corn Company, which later became Pioneer Hi-Bred, Secretary of Agriculture, Secretary of Commerce, and Vice President of the United States in the administrations of Franklin D. Roosevelt.

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An important question regarding these earlier, and even, current crop simulation models is why do some models seem to survive, in one form or another, while other models are relegated to library shelves and not used. The many reasons for this latter response may provide some insight to those who want to develop new or improve existing models. Reasons include: inadequate or non-existent model documentation, the code is very difficult to follow and modify, the model has limited applicability with respect to environment or cultivar, the inputs are difficult to obtain, the developer of the model doesn't want to support the model, the model is not robust and crashes often, over selling of a model's capabilities, and the model just doesn't work well; there are consistently large differences between simulated results and observations.

Whether we are conscious of it or not, we tend to have a philosophy about how we approach our disciplines, and perhaps even life itself. The following seems appropriate for crop simulation modeling. "Only the most naïve scientist believes that the perfect model is the one that perfectly represents reality. Such a model would have the same drawbacks as a map as large and detailed as the city it represents, a map depicting every park, every street, every building, every tree, every pothole, every inhabitant, and every map. Were such a map possible, its specificity would defeat its purpose: to generalize and abstract." (GLEICK, 1987). Thus, crop simulation modeling requires the ability to synthesize complex biological and physical interactions in a relatively simple, yet meaningful way. While most everyone will agree with the statement attributed to Albert Einstein "Make things as simple as you can, but no simpler", there probably will be contentious discussions about what is meant by "simple". Thus, one can find a range of algorithms representing the same process with different degrees of detail. Given this choice, a valid question would be, which is the best algorithm? A justified Socratic response would be, what is the problem, what are the available resources to address the problem? (Excellent examples of simplicity can also be found in works of art, where a single line or a bar of music can evoke powerful emotions, or in the elegant design of common household objects.) We can think of crop simulation models as "... formalized collections of testable hypotheses about how environmental variations affect plant processes", JAMIESON et al. (1998). The applications of crop simulation models can fit into

three broad categories. The first category is to understand. If one has a different, perhaps unique, perspective on a process and then incorporates an algorithm based on this unique view into a new or existing crop simulation model; does the result increase our understanding and knowledge of this and other related processes? Is there an improvement in the simulated results when compared with observations? Will these results provide the basis for a series of field or controlled environment experiments to further understand this process? The second category is to ask "what if" questions. The type of "what if" questions can range from management issues (e.g., cultivar selection, sowing date, irrigation scheduling, and pest management) to climate change and plant breeding (SHORTER et al., 1991). These responses can form the basis for policy decisions and regulations (MATTHEWS et al., 2000). The final category is to predict yields for crops grown around the world for large-scale commercial operations, such as candy manufacturers and grain companies. Predictions for this last category can be supplemented by ground truth, satellite data, and the ability to update models with real time data.

Perspectives

The following simile may provide some insights and alert us to some potential pitfalls of crop simulation modeling. A crop simulation model can be like a large plate of spaghetti: (1) there are many ideas on what constitutes 'perfection'. One can argue that the best sauce for a plate of spaghetti is a plain marinara sauce, while someone else can argue equally well that the best sauce is a pesto sauce with lots and lots of garlic. Similarly, there may be several different models for a single crop, which is the best model? As noted above, the first response to this question is: what is the problem? (2) There are many non-linear interactions. By its very nature, a plate of spaghetti consists of a series of intertwined strands. Similarly, many plant processes are connected to other processes. For example, transpiration is related to root and leaf growth, plant available soil water, leaf area index, and the interception of solar radiation. (3) Some of these interactions are direct and some may be indirect and subtle. It is difficult to follow an individual strand of spaghetti from one end to the other end as it intertwines with other strands. There is a high probability that in moving a single strand of spaghetti;

in varying degrees, all the strands of spaghetti will move. Similarly, by changing a single input variable in a crop simulation model, the results may change, some simulated variables being more sensitive than others to the changed inputs. Some examples of input variables that can influence output variables are initial soil nitrogen content, initial soil moisture conditions, sowing date, and sowing depth. (4) Different ingredients can be substituted for the original ingredients and still produce a good plate of spaghetti, 'good' simulation results can occur from compensating errors. Thus, one must ask, "Am I getting the right answers for the right reasons?" What happens if one variable is over predicted (e.g., kernel number) and another variable is under predicted (e.g. kernel weigh), but when multiplied together they provide the "right" (yield) answer. Is this situation "good" or "bad"? Of course the answer depends upon what was the original question and the consistency of these compensating errors. (5) No matter how good, don't eat too quickly; no matter how excited about implementing a new idea, take your time to document and code in a logical manner. When a new idea pops into one's head, the desire is to quickly see if the idea has merit. Speed becomes more important than documentation or clarity of the code. If implementation of the idea has been successful, other ideas immediately appear and the excitement about the earlier idea is replaced by the challenge of a new idea. With a high degree of certainty, at a later date one will need to look at this code and if the code isn't well written with clear documentation, it will be difficult to follow, even for the person who wrote the code.

This last point raises some interesting questions about the role of a modeler; does the person developing the algorithms also write the computer code that implements the algorithms? The answer depends upon the modeler, the model, and modeling application. If the main, or sole, user of the model is the person who developed the model, then the modeler will implement and evaluate a new algorithm. This approach does not guarantee that the algorithm will be well implemented; a good modeler may not be a good programmer, even though the crop simulation model may produce accurate simulations. There may be a two-stage process if there are multi users of a model or if a series of models are dependent upon each other in a multidisciplinary effort. The new algorithm initially should be implemented and evaluated by the modeler who developed it, perhaps

in a simplified version of the simulation model. After the modeler has determined that the new algorithm is robust, then the modeler should turn it over to a programmer to ensure that the new algorithm fits into the existing structure of the simulation model, and if appropriate, interacts properly with other models. The resulting simulation model should then be reevaluated to ensure it responds as the modeler originally envisioned.

Ideas and directions

How can one get ideas about developing new or modifying existing algorithms of plant related processes in response to a new need? Keeping abreast of the literature, attending scientific meetings, and discussing ideas with colleagues would be typical responses. Another approach, not used as often as it should be used, is to read or even reread classical scientific works in one's area of interest. An example is KIESSELBACH (1949), which deals with the anatomy and morphology of corn. The intended audience for this book was botanists, plant physiologists, corn breeders, and geneticists. The importance of this work is reflected in the printing of a special 50th anniversary edition by the Cold Spring Harbor Laboratory Press in 1998. Given current research trends to work on genetic scales of organization, this book details the cellular and organ level of organization, via drawings and pictures, and provides an overview of how corn grows and responds to the environment. The success of this book can be attributed to Kiesselbach's keen sense of observation and inquiring mind. This same approach may be useful in generating new ideas for algorithms, i.e., closely following crop development and growth combined with a spark of creativity.

Another approach to generating new ideas is to ask ourselves are we making full use of existing knowledge? Have we done a thorough search of the literature? Is it possible to reinterpret published data to fit our modeling objectives? The following two algorithms, which were used to simulate kernel number in winter wheat, serves to illustrate these points.

Published data for the winter wheat cultivar Karl 92 (GIBSON and PAULSEN, 1999), relating kernels per spike to maximum temperature, from the beginning of anthesis to the beginning of the linear grain fill period (Zadok Scale, ZC = 61-70) was used

to develop a relationship for kernel set (the number of kernels that do not form due to high temperature). The original data are shown in Figure 1a, while a reinterpretation of the same data are shown in Figure 1b. While a straight line would be a good fit, in a statistical sense (Figure 1a); Figure 1b provides a biological explanation as well as a good fit. Up to a maximum temperature of about 25 °C, there is no decrease in kernel number, above this value; there is a linear decrease in kernel number due to higher temperatures. The y-axis can be scaled by the highest value in order to obtain a 0-1 response factor to higher temperatures. To extend this result to other cultivars, one would have to know the relative sensitivity of the unknown cultivar to Karl 92. For example, using independent data for the cultivar Arapahoe, a cut-off temperature of 28 °C was determined. The magnitude of this latter value was verified from discussions with a wheat breeder.

This kernel set algorithm was incorporated in the wheat simulation model, CERES-Wheat (RITCHIE and OTTER, 1985). CERES-Wheat was also modified to reflect newer knowledge about the simulation of kernel number. FISCHER (1985) proposed an idea that kernel number per unit area could be determined from a harvest index type concept, based on biomass accumulation starting at the time when the flag leaf was fully extended (ZS =48) and ending at 50% anthesis (ZS = 65); 50% of the above ground biomass accumulated during this time period is partitioned to the spike and multiplied by a unit conversion factor of 100 to obtain kernels per unit area. This idea was incorporated into the model AFRWHEAT (WEIR et al., 1984) and AFRCWHEAT2 (PORTER, 1993). JAMIESON et al. (1998) successfully evaluated and incorporated an algorithm based on this idea into the wheat simulation model Sirius. The results of this modification are shown in Figures 2a and 2b. The root mean square error using the original version of CERES-Wheat was 4,350 kernels m^2 , while with the modified model it was 2,657 kernels m⁻², a 64% reduction in root mean square error. Additional details on these modifications to CERES-Wheat are given in MORENO-SOTOMAYER and WEISS (2004).

A further approach to generating new ideas for future crop simulation models is to look at progress in other areas, areas that are very different from crop simulation models, for example, cars. Cars of the future will be the same as cars 100 years ago; common to both are engines, brakes, steering, chassis, etc. What will be different is the technology used in these components. For example, General Motors predicts that the car of 2020 will run off hydrogen fuel cells that will power motors for each wheel, there will be no hydraulic brakes, brakes will be controlled electronically, and there will be a skateboard type chassis, where different car bodies can be attached depending upon the planned uses of the vehicle. (For more information about these cars, use a search engine (e.g., www.google.com) with the key words "GM Hy-Wire". Also note that not all experts in the field of hydrogen propulsion agree with this 2020 assessment.) Future crop simulation models will simulate development and growth of leaves, roots, stems, and reproductive organs, in response to an everchanging environment, as do current models; the difference will be that many of the algorithms of these future models will be based on genomic knowledge. This area of research is just beginning. The



Figure 1. (a): Data are from Gibson and Paulsen (1999), their Figure 1c, with their regression line. The x-axis is maximum daily air temperature (°C) and the y-axis is the number of kernels per spike. (b): Reinterpretation of the data from Gibson and Paulsen (1999), their Figure 1c. The x-axis is maximum daily air temperature (°C) and the y-axis is the number of kernels per spike.

proceedings of the symposium "Crop modeling and genomics" which was published in the January/ February 2003 issue (volume 95, number 1, pages 1 -113) of the Agronomy Journal may provide some research ideas. The task of incorporating genomics into crop simulation models will be very difficult; even though genes may be identified, their roles may not be known or only partially known. One approach to incorporating genetic knowledge into crop simulation models would be to take a robust algorithm that works well at the organ level and to determine if genetic linkages can be found and quantified. As with any problem in this area, interaction with some one (or group) with the appropriate expertise in plant genetics is necessary. While this expertise is necessary, there also must be interest by the plant geneticists in using this knowledge in crop simulation models.



Figure 2. (a): Comparison of observed versus simulated values of kernel number m⁻² using CERES-Wheat (V3.0) for two contrasting cultivars of winter wheat, Arapahoe and Karl 92. The RMSE was 4350 kernels m⁻². (b): Comparison of observed versus simulated values of kernel number m⁻² using a modified version of CERES-Wheat for two contrasting cultivars of winter wheat, Arapahoe and Karl 92. The RMSE was 2657 kernels m⁻².

Another approach to incorporating genetic knowledge into crop simulation models would be to take a simple, well-documented trait (e.g., plant height in wheat) and see how changes in plant height are related to changes in other plant organs. This approach could be classified as a genomic/allometric type approach.

Let us continue with the car/simulation model analogy. In order to be a safe driver, it is not necessary to understand how the engine works or be able to do repairs, although one should recognize when the car is not functioning properly. I do not believe this analogy applies to crop simulation models. The scientist who uses a crop simulation model must not only be responsible for the quality of the input data, but must be able to explain the simulated results based on an understanding of the physical and/or biological basis of the many algorithms that constitute a model. Do these results make sense? If not, do the results reflect a weakness in the model or some new insights that will have to be verified by experimentation? The scientific user of a simulation model should understand the algorithms that comprise the model. Whether they should be able to follow the computer code, and where appropriate, modify the code is another question, which has been addressed earlier.

Just as a crop simulation model attempts to capture key processes in the soil-plant-atmosphere continuum, we must think of another continuum as a future direction for simulation modeling. Opposite in scale to genomics, will be the expansion of models from the field to the farm to the landscape scale, associated with environmental and ecological considerations.

Final thoughts

Crop simulation modeling has an important educational role and it should not be limited to graduate education. A course in this subject could be a capstone course for undergraduates in crop sciences who have an analytical approach to problem solving. Crop simulation modeling by its very nature has to integrate processes in the soil-plant-atmosphere continuum. By providing a student with an appreciation of these many interactions, hopefully it will lead to a greater understanding of the complex processes and interactions that constitute an agricultural ecosystem. This understanding may lead future generations to incorporate sustainability into their professional activities. Comparing field observations with simulated results could provide the basis for discussions on field variability, crop simulation model limitations, and statistical procedures. A similar approach can be taken with grades K-12. For the earlier grades, studying a single process, such as change in leaf length or plant height and plotting these results may provide a positive educational experience for many students. The students can be engaged in simple exercises, such as, based on previous measurements; can they predict the change in the measured quantity? And of course the students should discuss the reasons for their success or lack of success. The same project could be extended to older students where they plot the results, and then try to fit curves to these data points, and explain the results at a higher level of understanding, relative to the earlier grades. Other projects could study the change in soil water as plants transpire, based on the classical work of Briggs and Shantz (1914), where the major components of this project would be plants and a scale. Projects of this nature combine science, mathematics, and communication skills.

An article in the New York Times (In Brazil, All May Not Be As Relaxed As It Seems, May 20, 2003) about business in Brazil had the following comments "Brazil's business elite are probably 'the most flexible, the most versatile, the most imaginative and the most nonrigid in the world,' Mr. Stern said." The Brazilians themselves call this innate flexibility jogo de cintura, which literally means 'the waist game', but which perhaps would best be interpreted as the talent to keep the economic Hula-Hoop turning." So the question becomes how can we translate the concept of jogo de cintura from business to science? The key words in the above quotation are flexibility, versatility, and imagination, which can be synthesized into, intuition and creativity. The most important thing, we as scientists, bring to a problem is our minds. If we limit our perspectives, we limit the number of solutions. This synthesis means not to be afraid of mistakes, that mistakes are tools to enable a greater understanding of the problem under study, and to preserver. There seems to me, at times, an unjust concern about using the latest technology in solution of a problem, without a thorough, careful analysis of the problem. For example, a current important problem in crop simulation modeling is, as it was 40 years ago, how to determine partitioning of dry matter to above and below ground components in response to abiotic stresses (temperature, water, nutrients). The physical tools to carry out this research are relatively

simple: a shovel, a ruler, a scissors, and a scale. What is lacking is a robust hypothesis that can tie together cultivar responses to these stresses. Muito Obrigado.

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