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Perspectives

Crop, soil and farm systems models – science, engineering or snake oil revisited

Brian A. Keating*

Qld Alliance Agriculture and Food Innovation (QAAFI), University of Queensland and formerly Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia

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ABSTRACT

This “perspectives” article draws upon close to 50 years of experience in the development and application of crop, soil and farm systems models in pursuit of enhanced productivity and sustainability of agricultural systems. The scientific foundations and practical utility of such models have been questioned by some and this article shares the author's learnings around model development, testing and application in settings of applied agricultural research and development. The article concludes that provided a rigorous scientific approach is retained to model development, parameterisation and application, farm system models will remain essential in supporting effective agricultural research – in particular in addressing the 21st Century challenges of food security and sustainable development in the face of climate change.

1. Introduction

Keating and Thorburn (2018) and Jones et al. (2017) have recently reviewed the evolution of crop, soil and farm systems models – a journey that spans 150 years and has its roots in the earliest scientific endeavours to understand soil and environment controls over plant growth and development. Digital technologies have co-evolved with simulation methods over the last 75 years, with computing capacity and accessibility improving by mega orders of magnitude within a single professional career.

As an undergraduate student in the early 1970's I heard passing reference to models being used to augment crop physiology studies. Despite this, classical growth analysis and classical statistics were the stock tools of trade for agronomists and crop physiologists. Most Universities had a mainframe with card readers as data input devices but as students the closest we got to advances in digital technologies were mechanical calculators pre-configured to calculate sums of squares for ANOVA. Another decade was to pass before the first PC-DOS / MS-DOS PC's appeared around 1981 and as they say – the rest was history! Forty years later, upon retirement from CSIRO, I observed individuals running complex farming system simulations over continental or global land surfaces with daily or sub-daily time steps over century time spans.

While computing and programming technology is no longer a significant constraint to cropping systems simulation (this has probably been the case from the 1990's onward), one wonders whether the science that underpins these models and the expertise to enable their valid utilization has kept pace with the advances in computing power. This niggling concern over the scientific appropriateness of model use is not new. Close to 25 years ago, Passioura (1996) provocatively questioned whether the growing interest in simulation modelling was actually science, perhaps engineering or even “snake oil”. As an early career agronomist who was finding simulation models immensely useful in exploring productivity and sustainability constraints in climatically risky environments, Passioura's negativity over the utility and scientific validity of simulation models was a significant cause for concern. With the benefit of 25 years of hindsight, it is timely to revisit Passioura's warnings and assess their continuing relevance as we enter the decade of the 2020's.

Passioura (1996) Identified two major classes of model, namely; (i) mechanistic models built from physical and biological component knowledge and “looking upwards” towards higher orders of system complexity with aspirations for generality and scientific insight and (ii) empirical models statistically fitted to data with potential for engineering applications within the limited domain of the data. He concluded the former had generally failed to advance physical or physiological understanding largely because of limited understanding of system constraints at the higher orders of complexity. He acknowledged the latter were sometimes of practical utility within the domain of the data used to build the model, but generality beyond that domain was

* Corresponding author.
E-mail address: b.keating@uq.edu.au.

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limited.

Passioura reserved his strongest criticism for models that he saw fell between these two poles. That is, models that purported to be mechanistically based but where the mechanisms were founded on incorrect process knowledge and/or where parameters and functional forms were fitted to data without sound physiological or physical foundations. While not specifically identified, models like DSSAT (Jones et al., 2003) or APSIM (Keating et al., 2003a; Holzworth et al., 2014) that were gaining recognition and widespread use at the time might have been a target for this warning. These models are structured around the key plant-soil-environment processes yet there is a high degree of pragmatism and empiricism in the choice of any individual functional forms or any set of parameters for the functions.

So how relevant are Passioura's observations and warnings today with the benefit of 25 years of hindsight?

My personal view is that Passioura was justified in his warnings about the risks of simulation models crossing over into the domain of "snake oil" purveyors. I see this risk however being primarily associated with the *abuse* of such models, rather than model usage per se. A primary source of abuse was what de Wit (1970) first called *"the most cumbersome and subjective technique of curve-fitting that can be imagined."* That is, uninformed and inappropriate fitting of model parameters to a particular dataset without regard to the physical or biological foundations of these models. In other words, "getting the right answers for all the wrong reasons"! This is a futile exercise and is "bad science". Short-term or localised appearances of model utility will disappear as attempts are made to extend the model application to different circumstances.

A related concern has been an over-reliance on the notion of "validation". That is, the model has been shown to have predictive power over a particular independent dataset and hence it is "validated" and can be deployed elsewhere without question. A more appropriate view is that these models are evolving hypotheses of how key plant-soil-environment relations interact, always subject to continuing refinement and always "wrong" at some level, but still potentially "useful" in carefully established circumstances (sensu Box, 1976). The validation process I have been most comfortable with has been to continuously expose the model to new datasets that "stress test" its performance in new directions. Exploring the key individual functions (plant development, growth and yield, water and nitrogen dynamics in both plant and soil is fundamental to ensuring models "get the right answers for the right reasons". Any evolution of model structure, functional forms or parameterisation has to perform across the entire model testing database – not just on one new dataset.

The APSIM team developed the idea of "sensibility testing" to augment traditional validation procedures. This means we would look for evidence of whether the model "made sense" alongside the crop/soil insights of an expert physiologist, agronomist or hydrologist. Does the model predict summary relationships that these practitioners believe to be robust? Examples might include robust summary relationships such as the French and Schultz (1984) relationship between yield and water seasonal water supply, yield-plant density curves, N response curves, yield-grain protein curves etc. The fact that these summary relationships are NOT directly specified in the model yet can "emerge" from the combination of model predictions of individual processes and their interactions gives the model developer and user added confidence in the robustness of the model structure and specification. (see Holzworth et al., 2011 for more on sensibility testing and software process and testing in general).

The earliest development and application of crop and soil models arose from the engineering domain – more precisely the operations research domain in the early 1950s. The two pioneer Dutchmen, C.T. de Wit (crop models) and C·H.M. Van Bavel (soil water models) both trained under Prof. van Wijk from the Shell Laboratories, a pioneer in application of operations research principles to optimising distillation processes in oil refining (see Keating and Thorburn (2018) for more on that story).

The view of simulation models as engineering tools does not mean they cannot generate new understanding – particularly understanding of "emergent" properties of complex and variable systems. In fact, it is this correspondent's experience that the more complex the farming system and more variable the soil and weather environment, the greater are the prospects for "novel <u>systems</u> understanding" to be generated through the combination of experimentation and simulation modelling. Examples from the correspondent's personal experience include; insights of fertiliser use in subsistence farming systems (Keating et al., 1991, 1992a; McCown et al., 1992) and intensive sugarcane systems (Keating et al., 1997), insights on the leaching and deep drainage risks from dryland farming systems (Asseng et al., 1998; Keating et al., 2003a, 2003b), insights on drought frequencies for policy formulation (Keating and Meinke, 1998).

The issue of "parsimony" in model design and parameterization has continued to arise (Antle et al., 2014; Hammer et al., 2019). Passioura (1996) called for agronomic (engineering) simulation models to be "as simple as possible and especially have a small appetite for data" and deploy "simple robust empirical relationships between the main variables" where uncertainty exists in understanding of "mechanistic structure". Yet anyone who has a working knowledge of the complex components and interactions that shape a farming system will know the real world is far from simple and parsimonious! The notion of an "understanding" of mechanism is also a relative one – we may for instance have robust and useful predictions of crop biomass production without a full understanding of all the biochemistry and physics that control leaf photosynthesis. In this correspondent's experience, the <u>model should be as simple as possible *in the context of intended application*, but no simpler</u> (a concept often attributed to Albert Einstein but not well authenticated).

Take for instance, the well-known simple model of French and Schultz (1984) which relates grain yield to seasonal rainfall. This provides valuable predictions of yield in the absence of any other information, but these predictions are certainly improved if there is some knowledge of soil water storage to elaborate the model. Further improvements can be made with knowledge of the crop life-cycle and a daily water balance replaces the seasonal water balance. When we took the CERES Maize model to Kenya for the first time, we found crops would not die under extreme water stress in the model yet we were observing that in practice (Keating et al., 1992b). Hence, given our interest was in the riskiness of cropping, it was critical that we elaborated the model to predict the crop death that was likely in about 5–10% of seasons in that environment. All these elaborations increase the numbers of functions and parameters in a model. Yet, they also add greater bio-physical realism and relevance to our systems investigations. The trade-off will always be a judgement call but what is critical is a robust process in model development, elaboration, testing and validation (see relevant comments above).

In my view Passioura was too pessimistic over the potential for what might be called the mixed functional/empirical models. Certainly usage patterns of models such as DSSAT and APSIM don't support any waning in interest in such models – in fact the reverse is true with a seven-fold increase in papers making use of the APSIM and DSSAT models between the years 2000 and 2015 (see Keating and Thorburn (2018)).

Model use per se does not necessarily imply positive impact. A good case study of impact can be found in the work on improving water use efficiency in wheat-based systems from southern Australia. In that work, simulation modelling was used in both pre-experimental and extrapolation modes at scales from plant to crop, system and nation. The potential for significant gain in paddock-scale yields through synergies of pre-crop and in-crop agronomic interventions was predicted by pre-experimental modelling (Kirkegaard and Hunt, 2010) and subsequently validated in on-farm experiments over 5 years (Kirkegaard et al., 2014). The specific combination of strict fallow weed management and early-sown, slower duration "fast winter" wheat not only increased yield and WUE at paddock scale (Flohr et al., 2018), but also at farm-scale by moving the entire sowing program earlier (Hunt et al., 2019), with predicted national increase in wheat production of 7.1 Mt. pa (approximately 30% increase). Further refinements combining long-coleoptile varieties for reliable early sowing into stored water following legumes or fallow have recently been predicted to offer even further yield improvements (Flohr et al., 2019), and these await experimental confirmation. That work exemplifies the highly productive combination of informed simulation in the hands of systems agronomists.

2. Contemporary trends and looking forward

The existing reality and future prospects for a changing climate to impact (positively or negatively) on global agricultural systems has grown from a niche area of scientific inquiry in the mid'90s to a central challenge for all fields of science in 2020. Climate change poses a particular challenge to the crop and soil modelling community. On one hand, simulation models are more central to our scientific methods than ever as we are exploring agriculture under future climates and direct experimental observations are necessarily very limited (e.g., FACE experiments are expensive and restricted in scope and cannot capture the full system effects). On the other hand, our abilities to ensure the models are valid and sensible – and "getting the right answers for the right reasons" are much more constrained. Also the depth of our physiological understanding of plant response to elevated CO_2, higher temperatures and other climate extremes is inevitably more limited. So we need simulation models more than ever in the face of climate change but we have greater cause to be cautious about their validity and utility.

The application of "ensemble" model predictions is an interesting development in crop-soil modelling (Wallach et al., 2018) but it remains to be seen whether this is useful development or a distraction. Crop-soil models are predominately deterministic – given the same inputs they generate the same predictions. It is variability in soil and weather inputs that generate variability in model predictions. Two crop-soil models producing different predictions of crop performance under a future climate reflect different biological or physical mechanisms at work within the model structures. Both can't be correct and taking the mean of an ensemble of models may or may not improve accuracy of predictions. The argument for ensemble modelling approaches has more traction in modelling of global and regional weather systems given the more fundamentally chaotic nature of global circulation models (Tebaldi and Knutti, 2007) but I remain unconvinced the same case applies in farming systems simulation. In my view, directing energy into understanding why differences in model performance under climate change are arising and then gathering data and evolving model structures or parameterization would be a more useful way forward.

It is not only the climate and farming systems that have changed over the 40 years of my career, but also the human dimension of model development and application. In the 1980's, the classical career trajectory was for a young researcher to build a model as part of their PhD and then apply that and other models as part of a career directed at practical agronomy or other disciplines including crop physiology and breeding, soil physics and agro-meteorology. The models were quite limited in scope and the application process often involved model development to address new problem settings. The strength in this approach is that we had well trained and experienced agronomists or physiologists adding models to their tool-kit. The good researchers retained a healthy scepticism for model output and took great care to ensure model parameterisation and application was scientifically robust. Today, it is possible to download very powerful and comprehensive modelling platforms (e.g. APSIM or DSSAT) from the web and for individuals to run these models with relative ease – essentially as a black box. But that does not mean the model applications are always scientifically sound and the interpretations robust. Those still active in support for such big model platforms (e.g., the software engineers on the APSIM Initiative) tell me that a lot of their effort goes into trying to build "workflows" and IT solutions including machine learning and automation that allow "users" to do "modelling". They lament the over-abundance of "users" and scarcity of "modellers or developers". I would add that the combination of practical agronomy and modelling competencies is even more scarce. Why might that be given the good examples of success? Are the skill sets inherently incompatible or is it a matter of our professional training and career regimes that discourage these cross-over competencies?

3. In summary

I have had the good fortune to train as an agronomist/crop physiologist in the pre-digital era and to have discovered the power of crop-soil simulation modelling early in a career directed at practical agronomic problem solving. Working on complex farming systems issues in regions of high climatic risk has stimulated my appreciation of the power of well-developed and well-applied simulation tools. I have not been backward in seeing this approach as agronomic engineering, built upon the foundations of scientific principles and understanding. I can appreciate Passioura's warnings of models in the context of "snake-oil salesmen". This warning is as relevant in 2020 as it was in 1996. However, I see this as a risk that can be managed with a rigorous scientific approach to model development, parameterisation and application. A healthy scepticism of model output and relentless pursuit of getting the "right answers for the right reasons" is part of this rigorous approach.

In 2020 with models critical to our addressing climate change challenges, I would look to our profession for the highest possible standards of scientific integrity in our modelling studies. Modelling climate change impacts, adaptation and mitigation options is essential, but there are many limitations in our models and in our understanding of these impacts and options and we need to address these uncertainties explicitly.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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