Simulation Models: Science, Snake Oil, Education, or Engineering?

John B. Passioura*

ABSTRACT

Crop simulation models can be divided into two groups: those that aspire to improve our understanding of the physiology and environmental interactions of crops (*science*), and those that aspire to provide sound management advice to farmers or sound predictions to policy makers (*engineering*). These quite different aspirations require quite different models. Scientific models are mechanistic. With a few exceptions, they have failed to meet their aspirations. They are typically flawed by being based on untestable guesses about the processes that control growth. They may, however, provide useful self-education for their developers. The best engineering models are based on robust empirical relations between plant behavior and the main environmental variables. Because of their empirical nature, we should not expect them to apply outside the range of the environmental variables used in their calibration. Within their calibrated ranges, however, some have proved useful in providing sound management advice. It is hard to see a useful role, other than self-education, for models that fall between the scientific and the engineering types.

Most members of the American Society of Agronomy probably think of themselves as agricultural scientists. The Dutch, however, who are a very practical people, call their graduates in agriculture *engineers*. I think that much of the debate that surrounds the use of simulation models in agriculture arises from confusion about the difference between science and engineering. Science is about discovering how the world works. Engineering is about solving practical problems (Fig. 1). The mode of thinking is different. In the profession of agronomy, in which engineering and science are closely intermingled, the tension between the two approaches is often very evident. The same tension appears in ecological analysis (Hauhs, 1990) and in hydrology (Klemeš, 1986).

THE ESSENCE OF ENGINEERING

Engineers typically apply set procedures to solve their problems. These procedures started out as rules of thumb, and have evolved over the years into books of tables and, with the advent of computers, into software packages, but in spirit they remain the same. The practitioners usually do not have much interest in questioning their rules of thumb. They want to get on with the job of applying them. While they may adjust these procedures in response to experience and the ever-present imperative to cut costs, only catastrophes like the failure of a structure stimulate them to question their procedures fundamentally, and to invoke the recursive flow of information depicted by the dotted arrow in Fig. 1. Inventions may also stimulate the flow towards theory, as in the classical example of the steam engine, which stimulated the development of thermodynamics.

CSIRO, Div. of Plant Industry, GPO Box 1600, Canberra 2601, ACT, Australia. Presented at a symposium, Use and Abuse of Crop Simulation Models (jointly sponsored by Div. A-3, the Computer Software Applications Committee, Div. C-2, and Div. S-1), at the ASA-CSSA-SSSA annual meetings in Seattle, WA, 14 Nov. 1994. Received 23 June 1995. *Corresponding author (Email: j.passioura@pi.csiro.au).

Published in Agron. J. 88:690–694 (1996).

An amusing example of the persistence of an erroneous rule of thumb comes from one developed by the ancient Romans for calculating the flow rate in an aqueduct: the unit of discharge was defined in terms of the cross-sectional area of the aqueduct occupied by water, but not in terms of the slope, and was used for hundreds of years (Philip, 1986). Presumably, it worked, at least most of the time, because the practitioners unconsciously kept the slope reasonably constant, but without saying so explicitly; they had developed the tacit understanding of their jobs that comes from apprenticeship. The lack of explicit understanding led to puzzles and anxieties, however, and the occasional search for fictitious water thieves, when the cross-sectional area of the water entering a section of aqueduct of small slope failed to be matched by the cross-sectional area of that leaving the section where the slope was larger. Despite such anxieties, the rule of thumb remained unchallenged for centuries.

I do not mean by this example to disparage the use of rules of thumb. In general, those that persist do so because they work. At their best, they represent robust empirical relationships on which we are prepared to stake our lives. Another well-founded hydrologic example comes from a Canadian hydrologist, Vit Klemeš, who has pointed out that the 19th century railway engineers used to decide the height at which to build a bridge over a river by searching for the highest flood mark they could find and making the bridge a little higher than that. He argues that decades of allegedly scientifically based hydrologic modeling has failed to produce flood prediction models that are noticeably better than this simple rule of thumb (Klemeš, 1982; V. Klemeš, personal communication, 1995).

THE STRUCTURE OF CROP SIMULATION MODELS

From about 1970, when computers became easily available to help us deal with the complexity of crops, the craft of crop simulation modeling developed rapidly. Two distinct types of model emerged: one was essentially practical, and combined a few rules of thumb to predict the behavior of crops. The other was seemingly scientific in spirit, and sought to represent the biological and physiological processes thought to occur in plants and their environments (Passioura, 1973). These two approaches correspond to what Addiscott and Wagenet (1985) termed *functional* and *mechanistic* in their analysis of leaching models, although their terminology has not proved popular, perhaps because there seems to be a code of honor among most simulation modelers that decrees that only mechanistic models are worth producing. Is, for example, a routine for calculating the rate

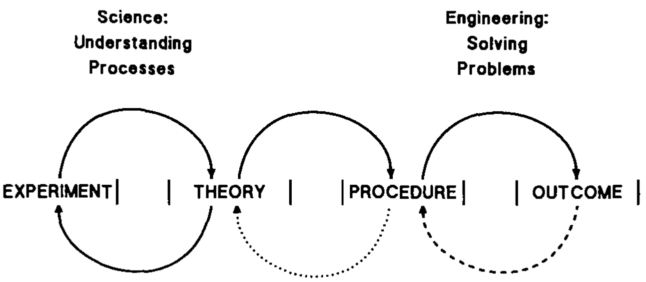

Fig. 1. Loops illustrating how science and engineering differ and interact. The solid arrows are the norm, the dashed one signifies responses to engineering experience, and the dotted one to engineering failures or inventions. Science is concerned with developing views about how the world works (e.g., theory, laws) and with explicitly testing those views (e.g., by experiment, focused observation). Engineering is concerned with achieving particular practical outcomes by using set procedures that are typically based on a mixture of well-established theory and robust empirical relationships.

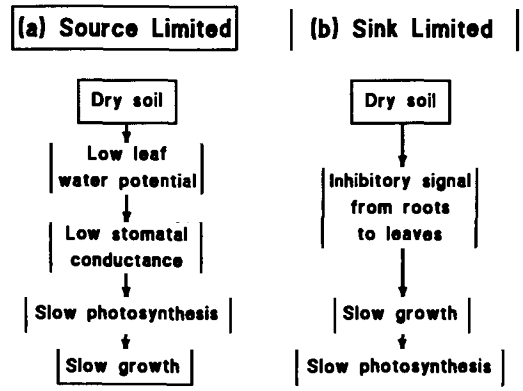

Fig. 2. Two scenarios of markedly different structure that depict how the growth of droughted plants may be controlled.

of plant development that is based on a correlation with degree-days mechanistic or functional? Perhaps the answer does not matter. However, the difference in intent implicit in the terms science and engineering in Fig. 1 does matter.

The range in complexity among models remains large, but the spectrum has been filled in by a plethora of models of various degrees of complexity and purpose. It seems to me, though, that most currently effective crop simulation modeling is closer in spirit to an engineering exercise than to a scientific one. Good science involves developing a set of views about the world that are subjected to penetrating experimental (or observational) testing, but crop simulation models are largely untestable in this sense. We are honest enough to have adopted the word *validation* for the process of comparing the output of a model with a new dataset. The inevitable disagreement usually leads us to adjust the parameters in our models, rather than to examine their structure, thus ensuring that we remain in the right-hand loop of Fig. 1. Changes in structure typically come from explicit experimental work, aimed at testing well-defined hypotheses, as depicted in the left-hand loop, although some structural insights have come from simulation models, as I discuss below.

What do I mean by *structure*? The following example illustrates the idea. Many of the mechanistically based simulation models use photosynthetic rate as the central variable for determining the growth rate of a crop. The photosynthesis is determined by many other variables, one of the most important of which is stomatal conductance. If the crop starts to experience water stress, it is supposed that the leaf water potential falls, in a way that can be calculated in terms of the transpiration rate and the hydraulic resistances within plant and soil, and this in turn induces stomatal closure and reduced photosynthesis. This conceptual structure is essentially that devised by Cowan (1965) many years ago, in which for the first time he combined the work of Gardner (1960) and others on the flow of water to roots with a simple algorithm for relating stomatal conductance to leaf water potential. This structure, depicted in Fig. 2a, may often be true where low leaf water potentials are induced in well-watered plants by very large evaporative demands. A particularly clear example of such circumstances, at least for the connection between leaf water potential and stomatal conductance, is provided by the study of Saliendra et al. (1995) on a riparian species. However, a simulation model based on Fig. 2a can be made to fit the data even where the structure is not true. Applying the model does not challenge this structure.

An alternative view of the relation between photosynthesis and growth in a water-stressed plant is that the plant senses that its environment is deteriorating, and determines its growth rate accordingly. In this scenario, photosynthetic rate does not determine the growth rate of the plant. The reverse is true: the growth rate determines the rate of photosynthesis. In the parlance of carbon-partitioning physiologists, the plant is sink limited rather than source limited. In fact, there is a spectrum of circumstances, ranging from complete sink limitation to complete source limitation. Many pieces of evidence are available to suggest that plants growing in inhospitable soil are largely sink limited, and that the root system responds to the soil conditions by generating a signal, probably hormonal, that is transmitted to the shoot, as depicted in Fig. 2b (Barlow, 1986; Passioura, 1988; Davies and Zhang, 1991; Masle, 1992). Now if this structure is true, a model based on an entirely source-limited model can never be relied on to work, and the calibration of it against a given data set is, in de Wit's (1970) devastating words, "the most cumbersome and subjective technique of curve-fitting that can be imagined." It is notable that the well-established CERES family of crop models, which are predominantly functional rather than mechanistic, implicitly favor this second scenario in that they relate transpiration and growth to soil water content rather than to leaf water potential. SIMTAG (Stapper and Harris, 1989), an effective model of water-limited wheat (*Triticum* spp.) in a Mediterranean environment, also implicitly favors this second scenario.

An example from soil physics that matches the physiological example of Fig. 2 is that of infiltration and redistribution of soil water. Many modelers assume that the flow is one-dimensional, and seek to improve the accuracy of their predictions by measuring the appropriate parameters, for example those defining hydraulic conductivity, with increasing spatial resolution. If the flow is occurring preferentially, however, for example in continuous macropores, or if there are perched water tables that result in lateral flow in the soil, then the one-dimensional model is inappropriate, and persisting with it while increasing the level of spatial detail is futile.

It is in the realm of environmental physics, though, that we probably do know enough about the structure of the main processes for us to be reasonably confident of our predictions, at least where they concern the aboveground microenvironment within crop canopies. A good example of success in this area is that of Berry et al. (1991), whose simulation of the environment close to the surface of transpiring corn (*Zea mays* L.) leaves gave good insights into the interactions between prey and predator mites.

Reynolds and Acock (1985), following R.V. O'Neill, have discussed sources of error in relation to the complexity of models. They dissected the notional total error into two components, one arising from errors in estimating parameters, the other arising from systematic bias resulting from oversimplifying. They postulated that cumulative errors in the parameters grow with the number of the parameters as a model becomes more complex. And they postulated that this systematic bias (which is similar to what I have been calling erroneous structure) decreases as complexity increases. Figure 3a, adapted from their Fig. 5 illustrates this argument. Their argument is convincing where we are sure of the fundamental structure of the system—for example, adding a wing mirror to the simulated model of a car will improve our prospects of predicting the overall aerodynamic drag. The aerodynamic principles are well understood. However, if the structure is fundamentally wrong, as it could be in the example of photosynthetically driven growth illustrated in Fig. 2, then no amount of complexity will improve the structural error. There will be an irreducible minimum error, as illustrated by the dotted asymptote in Fig. 3b.

Occasionally, though, the structure seems to be so wrong that no amount of adjusting of the parameters enables the model to fit the data. When that happens, we have moved beyond the realm of validation and are in a position to discover something new. A good example is the problem that the CERES models met with their routine for the withdrawal of water from the subsoil (J.T. Ritchie, personal communication, 1983). This routine greatly overestimated the rate of uptake by the roots, even when the measured root length density was used. The disagreement stimulated research into alternative structures for the routine: for example, that the roots were not uniformly distributed through the given layer of soil, but were clumped into preexisting pores or cracks (Passioura, 1991).

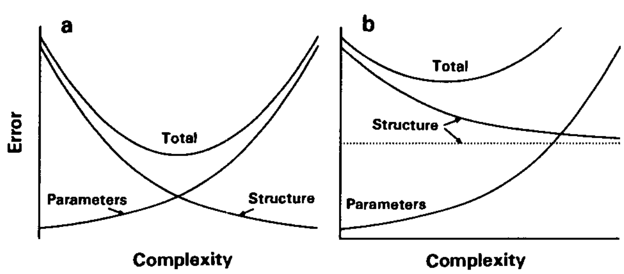

Fig. 3. Notional components of prediction error in models of increasing complexity: (a) when the structure of the system is well understood; (b) when the structure is wrong, with the irreducible structural error represented by the dotted asymptote (after Reynolds and Acock, 1985). Complexity and error increase away from the intercept.

Another example comes from Loomis et al. (1976), whose sugar beet (*Beta vulgaris* L.) model failed when they changed plant density, owing to its having the wrong structure for partitioning assimilate between root and shoot. This failure stimulated work on reciprocal grafts between beet (large root, small leaves) and chard (small root, large leaves) that showed that the voracious appetite of a small fraction of the cells in the root of the beet largely determined the size of the axis (Rapoport and Loomis, 1986).

Even if the structure is right, as it might be in some of the leaching models when they are applied to soils in which the flow is essentially one-dimensional, the models can rarely be applied with confidence to a field, because the parameters vary greatly in space. We have to assume average values of, say, the hydraulic conductivity to apply the Richards equation, and because this equation is not linear, the averaging is an art rather than a well-defined procedure, and often works poorly.

EDUCATION

So far, the part played by the large mechanistic simulation models of crops, those that aspire to occupy the scientific end of the spectrum, seems to have been largely one of self-education for the developer. Perhaps this is inevitable: these models are typically so complex that nobody but the developer is likely to have the enthusiasm to dip inside them. Thus, they are not transmissible to others in the sense that the research described in a typical research paper is transmissible. We do not know enough about the structure of the soil-plant-atmosphere system to expect such models to be accurate, except perhaps in the domain of the aboveground microenvironment. They are too complex to be tested as entities, but talented developers enhance their understanding of the interactions that occur and that may be far from obvious. The formidable understanding of the interacting processes within plants, or between plants and their environment, that is evident in the writings of, for example, R.S. Loomis or J.M. Norman, has undoubtedly been honed by their developing mechanistic simulation models (see, for example, Loomis and Connor, 1992; Norman, 1989). At best, comprehensive mechanistic models of crops give structural insights to their developers. At worst, they are merely time-wasting ceremony. There is little point, for example, in trying to cope with the structural difficulty illustrated in Fig. 2 by creating a simulation model that combines both scenarios. Such a model would merely be an elaborate shopping list of disposable parameters having no predictive value.

Mechanistic models are increasingly being used as teaching tools. This use may be economical—fewer teachers are required—but is alarming for the reasons cogently argued by Philip (1991): there is a great danger that students who are so taught, and who are not in a position to question what the program is doing, will graduate believing that what they have seen on the computer screen is the truth—unless they have been thoroughly exposed to real as well as to simulated plants. Fantasies in FORTRAN can too easily become fact.

Perhaps the most promising use of simulation models as teaching aids is in educating farmers. Good farmers are generally good observers of what is happening in their fields, and involving them with models, at least models with an easily satisfied thirst for data, may make them even better observers. The SIRATAC model for guiding integrated pest management in cotton (*Gossypium* spp.) eventually outlived its usefulness because the participating farmers became such talented observers that they could make appropriate tactical decisions without the use of the model (Hearn and Brook, 1989; A.B. Hearn, personal communication, 1995).

REALM OF APPLICABILITY

If few crop simulation models are clearly at the scientific end of the spectrum with engineering at the other, then there is not much point to the rest unless they are useful in some practical sense. How effective can we expect them to be? If they are based essentially on rules of thumb—empirical relationships established in a given environment—there is little reason to expect that these relationships will apply outside that environment. An essential requirement for a good working crop model is that it be able to predict yield with reasonable accuracy throughout the range of variables over which it was calibrated. If it can do that, then it can usefully provide both strategic and tactical advice. An example of strategic use is given by Hearn's (1994) cotton model, OZCOT, which has been calibrated for a given restricted irrigation area and which can be used to decide what area of cotton to grow in dry years when irrigation water is restricted (Dudley and Hearn, 1993). For example, if only half the normal water supply is available, the model can give good advice on whether it is better to grow, say, only half the normal area of cotton and give it the normal amount of irrigation, or to grow the normal area with only half the normal amount of irrigation.

What is especially alarming is the use of models outside the range over which they have been calibrated, as for example in trying to assess the response of crops to scenarios concerned with global atmospheric change. Trouble is sure to arise, not only because we are extrapolating beyond our calibrating dataset rather than interpolating within it, but also because the processes that we are trying to model are generally nonlinear, so that interactions between them can often lead to unexpected results. To claim that we can predict what will happen is disingenuous.

A fascinating example of the influence of nonlinear interactions comes from a study of the AFRCWHEAT model for a range of scenarios predicted by three general circulation (GCM) models (Marshall et al., 1996). The model was used in two ways for four sites. Although the GCMs all produced roughly similar scenarios in relation to annual averages of climatic variables (e.g., in predicting changes in average temperatures), they gave different estimates of variability on a monthly scale. When AFRCWHEAT was run using synthetic weather generated by each of the GCMs for the year 2050, it predicted a slight decrease in yield, of about 2%, for each of the four sites. However, when it was run using synthetic weather generated from a composite scenario of the climate, obtained by averaging the predictions of the GCMs, AFRCWHEAT predicted a substantial increase in yield, of about 10%, at every site. In these nonlinear systems, the order in which one does any averaging can profoundly affect the outcome. Nonhebel (1994), in a similar analysis, showed large differences in the output of a crop simulation model depending on whether actual daily weather data were used as input over a run of years, or whether synthetic daily data were used, calculated as averages from the same run of years. Russell and van Gardingen (1996) have highlighted the problem of the large variation in actual yield within an apparently uniform field. They cite an example of wheat yield data collected at a scale of tens of square meters with a recording harvester; the yield ranged from 4.5 to 8.0 t ha^{-1} and averaged 6.6 t ha^{-1}. Can we be confident that average inputs for soil properties will accurately predict the average yield for such a field?

CONCLUDING REMARKS

There is much that we do not know about the mechanistic structure of the workings of plants and their interactions with their environment. As crop physiologists and agronomists, we are faced with two main challenges: to illuminate those hidden structures—a scientific challenge; and to make use of what we do know to improve the management of agricultural enterprises—an engineering challenge. It is important to distinguish between the two. While we remain ignorant of essential structures, it is futile to develop mechanistic simulation models to help manage farms that are based on guesses about these structures. To claim that we know these structures when we do not gives us something in common with snake oil salesmen. Perhaps the best that could be said in our defense in such circumstances is that, to paraphrase Medawar's (1967) remark about Teilhard de Chardin: Before deceiving others we had taken great pains to deceive ourselves.

What I think we have learnt about agronomic (engineering) simulation models so far is that they need to be as simple as possible, and especially that they must have a small appetite for data; that, where we are not totally confident of the mechanistic structure, they should be based on simple robust empirical relationships between the main variables; and that, given this empirical nature, we should not expect, or claim, that they will be applicable outside the conditions in which the empirical relations were established. The overall aim is accurate prediction on which to base sound advice. In contrast, the aims of the best scientific simulation models are qualitative. We are looking for illuminating comprehensive failures that will stimulate us to change the way we think about the workings of the crop and its interactions with its environment. Confusing the two aims leaves us floundering.

ACKNOWLEDGMENTS

I am indebted to the many colleagues with whom I have had stimulating discussions about simulation modeling. Many of these colleagues are referred to in the text. Of those not already thus acknowledged, I particularly thank Peter Gillard and Ian White.

REFERENCES

Addiscott, T.M., and R.J. Wagenet. 1985. Concepts of solute leaching in soils: A review of modelling approaches. J. Soil Sci. 36:411–424.

Barlow, E.W.R. 1986. Water relations of expanding leaves. Aust. J. Plant Physiol. 13:45–58.

Berry, J.S., T.O. Holzer, and J.M. Norman. 1991. Experiments using a simulation model of the Banks grass mite (Acari: Tetranychidae) and the predatory mite *Neoseiulus fallacis* (Acari: Phytoseiidae) in a corn microenvironment. Environ. Entomol. 20:1074–1078.

Cowan, I.R. 1965. Transport of water in the soil-plant-atmosphere continuum. J. Appl. Ecol. 2:221–239.

Davies, W.J., and J. Zhang. 1991. Root signals and the regulation of growth and development of plants in drying soil. Annu. Rev. Plant Physiol. Plant Mol. Biol. 42:55–76.

de Wit, C.T. 1970. Dynamic concepts in biology. p. 17–23. *In* Prediction and measurement of photosynthetic productivity. Proc. IBP/PP Tech. Meet., Trebon. Pudoc, Wageningen, Netherlands.

Dudley, N.J., and A.B. Hearn. 1993. Systems modeling to integrate river valley water supply and irrigation decision making under uncertainty. Agric. Syst. 42:3–23.

Gardner, W.R. 1960. Dynamic aspects of water availability to plants. Soil Sci. 89:63–67.

Hauhs, M. 1990. Ecosystem modelling: Science or technology? J. Hydrol. 116:25–33.

Hearn, A.B. 1994. OZCOT: A simulation model for cotton crop management. Agric. Syst. 44:257–299.

Hearn, A.B., and K.D. Brook. (1989). A case study of the application of a knowledge-based system to cotton pest management: A tale of two technologies. AI Applic. Nat. Resour. Manage. 3:60–64.

Klemeš, V. 1982. Stochastic models of rainfall–runoff relationship. p. 139–154. *In* V.P. Singh (ed.) Statistical analysis of rainfall and runoff. Water Resources Publication, Littleton, CO.

Klemeš, V. 1986. Dilettantism in hydrology: Transition or destiny? Water Resour. Res. 22:177S-188S.

Loomis, R.S, and D.J. Connor. 1992. Crop ecology: Productivity and management in agricultural systems. Cambridge Univ. Press, Cambridge.

Loomis, R.S., E. Ng, and W.F. Hunt. 1976. Productivity of root crops. p. 269–286. *In* R.H. Burris and C.C. Black (ed.) CO_2 metabolism and the productivity of plants. Univ. Park Press, Baltimore, MD.

Marshall, B., J.W. Crawford, and J.R. Porter. [1996]. Variability and scaling: Matching methods and phenomena. *In* P.R. van Gardingen et al. (ed.) Scaling-up. Cambridge Univ. Press, Cambridge (in press).

Masle, J. 1992. Will plant performance on soils prone to drought or with high mechanical impedance to root penetration be improved under elevated atmospheric CO_2 concentration? Aust. J. Bot. 40: 491–500.

Medawar, P.B. 1967. The art of the soluble. Methuen, London.

Nonhebel, S. 1994. The effects of use of average instead of daily weather data in crop growth simulation models. Agric. Syst. 44: 37–396.

Norman, J.M. 1989. Synthesis of canopy processes. p. 161–175. *In* G. Russell et al. (ed.) Plant canopies: Their growth, form, and function. Soc. Exp. Biol. Semin. Ser. 31. Cambridge Univ. Press, Cambridge.

Passioura, J.B. 1973. Sense and nonsense in crop simulation. J. Aust. Inst. Agric. Sci. 39:181–183.

Passioura, J.B. 1988. Root signals control leaf expansion in wheat seedlings growing in drying soil. Aust. J. Plant Physiol. 15:687–693.

Passioura, J.B. 1991. Soil structure and plant growth. Aust. J. Soil Res. 29:717–728.

Philip, J.R. 1986. Frontinus, Leonardo, and you. p. 44–48. *In* Ockham's razor. Australian Broadcasting Corp., Sydney.

Philip, J.R. 1991. Soils, natural science, and models. Soil Sci. 151: 91–98.

Rapoport, H.F., and R.S. Loomis. 1986. Structural aspects of root thickening in *Beta vulgaris* L.: Comparative thickening in sugarbeet and chard. Bot. Gaz. (Chicago) 147:270–277.

Reynolds, J.F., and B. Acock. 1985. Predicting the response of plants to increasing carbon dioxide: A critique of plant growth models. Ecol. Modell. 29:107–129.

Russell, G., and P. Van Gardingen. [1996]. Problems with using models to predict regional crop production. *In* P.R. van Gardingen et al. (ed.) Scaling-up. Cambridge Univ. Press, Cambridge (in press).

Saliendra, N.Z., J.S. Sperry, and J.P. Comstock. 1995. Influence of leaf water status on stomatal response to humidity, hydraulic conductance, and soil drought in *Betula occidentalis*. 196:357–366.

Stapper, M., and H.C. Harris. 1989. Assessing the productivity of wheat genotypes in a Mediterranean climate, using a crop-simulation model. Field Crops Res. 20:129–152.