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Introduction

Modelling cropping systems—highlights of the symposium and preface to the special issues

1. Introduction

Science has developed and applied models for centuries, but automated calculations based on program instructions have emerged only during the last few decades. Agronomic models condense assumptions about biological process interacting with the physical and chemical environment through mathematical equations. The process of developing models to simulate the crop-soil interactions driven by weather and agricultural management has been ongoing for more than three decades. The goal to evaluate agriculture and the associated impact on economic, environmental and human health related aspects has lead to the development of models that simulate the behaviour of complex cropping systems. After great scientific progress and expectations in the first two decades, there now is new a widespread feeling that we face new challenges and prospects, both in terms of science, simulation techniques and application.

The 2nd International Symposium on Modelling Cropping Systems, held in Florence, Italy, from 16 to 18 July 2001 (Bindi et al., 2001), addressed questions concerning agricultural modelling such as (i) are we making progress in crop modelling? Can we do better? (ii) when is a model adequate? (iii) why are you modelling? Applications and user interaction, and (iv) which software designs are needed for evolution? These essential questions reflecting the awareness of the sketched dilemma in agronomic science were addressed in four sessions that all contained a start-up panel discussion, a series of oral and poster presentations with short discussions and a final plenary discussion. Some highlights raised during the symposium are discussed below.

2. Session A. Approaches for process simulation

Are we making progress in crop modelling? Can we do better?

J.R. Porter (chair)[a], G.L. Hammer[b], T.R. Sinclair[c], M.J. Kropff[d]

[a]Department of Agricultural Sciences, KVL, Denmark; [b]APSRU, Department of Primary Industries, Toowoomba, Queensland, Australia; [c]ARS-USDA, Gainesville, FL, USA; [d]Crop and Weed Ecology group, Wageningen University, The Netherlands

The purposes of modelling dictate the criteria for measuring advance. Two major purposes for crop modelling are to improve scientific understanding of crop and cropping processes and to predict the consequences of cropping system manipulation. Scientific understanding in this area springs from the synthesis of isolated phenomena by the dynamic and integrative framework of crop modelling or from the hypotheses generated in dissecting understanding of responses at the integral crop level using such a dynamic framework. Prediction is part of problem solving and prediction and analysis of crop management

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interventions are often enhanced via simulation and crop models that generate a platform for the dialogue required for progress. Modelling is now seen as a natural component of the toolbox of crop science, a view that has emerged within the past 20 years. However and by definition, cropping systems models do not contain all the available knowledge about crops and soils but seek a simplified representation of reality. In common with experimental studies, the question is whether the degree to which models approach reality is close enough. Reality in cropping system models stems not just from the understanding and representation of biophysical reality, some aspects of which have been approached similarly in many models, but is increasingly being seen as including the human actors within agro-ecosystems. In seeking to assess progress in modelling we discuss understanding and prediction as two separate issues but then ask whether their separation is the main impediment to progress.

2.1. *Scientific investigation*

We argue that crop modelling has led to modest progress in our understanding of crop performance. Modelling has helped to understand the dynamic integration of processes underpinning crop and soil function and has, thereby, assisted progress in defining and understanding key physiological determinants of crop performance. This has been of major importance in assisting post-hoc understanding of crop function. There have been few examples of scientific innovation based directly on crop modelling; an exception has been the importance of non-linearity of crop response linked to climate variability. Modelling has also allowed alternative hypotheses of crop function, such as the determination of seed nutrient concentration, to be explicitly framed and hence tested.

This above view reflects the effort in modelling to date on major environmental and crop management influences. We anticipate that predicting gene(s) function in crop improvement will provide one emerging challenge for scientific investigations using crop models. This has already started with examples of the physiological basis and modelling of genetic variation in particular traits. The critical role for modelling lies in connecting gene networks to their consequences for phenotypic expression *within a cropping context*. Molecular biology, leading to information on the genetic architecture of 'traits', is progressing far more rapidly than the theoretical frameworks connecting genes, phenotypes and crops and we have not progressed conceptually beyond single gene systems and their protein products. We suspect that modelling will have a key role to play in scientific innovation and integration in this area. One of the initial challenges will be to develop relatively simple models of the action of gene networks that give clear indications of what might be expected from a modified genetic network within a cropping system. Another challenge will be how to utilise the crop physiological understanding embedded in crop models in a manner that helps plant breeders to utilise developments in molecular biology to improve breeding methods.

As well as assuming a potential role in integrating molecular genetics, we conclude that crop simulation modelling will diverge upwards from its present scale of interest and operation. It will broaden from the plant and cropping level to the wider agro-ecosystem level for studies and education in land use associated with environmental and ecological aspects of farming in a landscape. This mainly requires linking existing crop modelling capabilities and connections to the economic and social aspects of the broader system.

2.2. *Problem solving*

We think that a modelling approach is leading to progress in our ability to predict consequences of cropping system manipulation. Some modelling activities have reported levels of predictive capability that allow confident extrapolation through time in crop management. However, problem solving in the real-word that involves using models as tools, also recognises that social and economic factors often override the biological determinants of a decided course of action. This means that satisfying client demand and their expectations of a prediction for management must be placed within a larger framework of joint discussion.

The role of models here is to illustrate the consequences of alternate courses of action. Our final issue is whether the scientific development and problem-solving aspects of models can move forward simultaneously.

2.3. Separation or connection

There is a disparity of views on whether separating scientific investigation and problem solving impedes progress in crop modelling. Some would argue that scientific progress is related only to scientific investigation; others that scientific progress is enhanced via problem solving, with each informing the other. Acts of problem solving often expose weaknesses in understanding through lack of predictive ability, such as in soil-crop interactions. Thus, relevant management questions can act as one stimulus to the scientific improvement of models although this clearly also happens as a result of scientific curiosity. In other words, problem solving is not inimical to the goal of producing more scientifically interesting and complete crop models. Operationally, investment in generic software frameworks to facilitate the connection between process understanding and crop response prediction is needed for future progress, as discussed below in the introduction to session D. The key word is facilitation. In this we need to have intellectual understanding progressing at roughly the same rate as the technical developments for implementing models. We need to see a connection with practitioners, farmers, advisors and plant breeders, in problem solving as one way of generating progress in crop modelling in the future.

3. Session B. Model parameterisation and testing

When is a model adequate?

P.A. Leffelaar (chair)[a], H. Meinke[b], P. Smith[c], D. Wallach[d]
[a]Plant Production Systems group, Wageningen University, The Netherlands; [b]APSRU, Department of Primary Industries, Toowoomba, Queensland, Australia; [c]Department of Plant and Soil Science, University of Aberdeen, UK; [d]Unité d' Agronomie, INRA Toulouse, France

The simple answer to the question ‘when is a model adequate?’ is: ‘when the model satisfies its objectives’. This answer implies that we can unambiguously assess this satisfaction and that we explicitly know the objectives.

Objectives, ‘something towards which efforts are directed’ according to the Longman English College Dictionary, may, for instance, range from developing models for (i) summarising information about a system to deepen its understanding, via (ii) solving a practical problem, to (iii) conveying knowledge about a scientific problem to colleagues and students. Sometimes these objectives may be combined, particularly at early stages of model development, but ultimately different objectives require different models.

Adequacy, ‘the quality or state of being sufficient for a specific requirement’ according to Longman English College Dictionary, must be assessed by confronting the model behaviour with the objectives. The first problem we are faced with is, however, that our agronomic models usually comprise a mixture of rate equations, empirical relationships, and different aspects of soils and plants, and use irregular weather data, so that only numerical computer program solutions, rather than analytical mathematical closed solutions, can be obtained. Therefore, not the mathematical model representing the system is tested, but rather the computer program, with all its added technical bother and possible errors. This may lead to the situation that both theory and experiments are correct, but that they do not match because the calculations are wrong. Hence, *how to assess model adequacy?* Three major items play a role: system representation, program verification, and program validation.

3.1. System representation

A model represents a system in a simplified way. Depending on the objectives of the study, different simplifications may be made. For instance, in a soil-plant-atmosphere system one has possibly to consider belowground heterogeneity such as cracks, structural elements or aggregates, and hysteresis in the soil water characteristic, above ground heterogeneity such as light distribution in a row crop or in an agro-forestry system, and one has to decide whether a one, two or three dimensional model is best. The spatial and temporal scales of the model will result from these choices. In many agronomic studies to date homogeneous, 1D models are developed and used. If it is proven that this satisfies the objectives, nothing is wrong: the simplest model is generally preferable. The question often remains, however, whether introducing heterogeneity in modelling would contribute to a better understanding of the system.

The domain of application of the model should be established, by investigating the degree of overlap of the domains of application of the individual submodels, consisting of explanatory differential equations, descriptive relationships, parameters and forcing functions, such as the weather. Even if the model is initially in its domain of application, very often non-expert users too easily change parameter values to values outside their known range of variation. This is done during the calibration procedure when parameter values are selected in order to minimise the difference between estimated and measured variables. Conceptually, this degrades a process-based model to a statistical fit (Penning de Vries and Van Laar, 1982). Such a curve-fitting approach not only leads to parameter sets that can be completely erroneous when environmental conditions are changed, but it also gives the wrong impression that model performance is acceptable. This has caused a lack of stimulation in model improvement through testing and using different approaches for process simulation.

3.2. Program verification

Program verification is meant to check the correctness of the implementation of the model into a computer program (Van Waveren et al., 1999). To be able to trust the program of the model, we have a number of checks at our disposal. A good start is to check all units, rather than dimensions, in the program listing. This not only applies to equations, but also to the parameters. Using the SI system and one consistent set of units throughout the program listing prevents cumbersome errors. Beneficial use can be made of the laws of conservation of mass and energy to check the impossible production or disappearance of matter and energy in the program calculations. A very strong tool in investigating a program technically is so-called time step convergence. The time step of integration depends on the smallest characteristic time in the equations, but it is often hard to assess its value because of the many equations. However, it is possible to make model runs using each run a smaller time step and finally establish the time step for which the model outcome does not change anymore as compared to the previous run. Principally, an infinitesimal small time step would lead to the analytical solution, if existing.

3.3. Program validation

Program validation (although the term is rather controversial in the relevant literature) is the comparison of the model results with an independent set of measured data to determine how well the model performs (Van Waveren et al., 1999). Such a comparison is usually done at the system level and is thus the result of both the feedbacks within and between each of the composing submodels. Possible counteractions between (sub)model components can not be noticed, however. Therefore, validation should both take place at the level of subprograms and of the complete program (Leffelaar, 1990). Performing such a validation requires not only the proper tools and software design (Section 5), but also detailed data sets. Too often model validation is done using data which do neither have the detail nor the temporal resolution to perform such tests.

To assess agreement between data points and simulation results plots are currently made and judged qualitatively. There is a lack for standardised procedures for model evaluation. Most of the indices used are based on the difference calculated vs. measured, and there is very little quantitative attention for aspects related to the pattern of residuals and time series comparison. A source for misleading comparative evaluation of models can be evaluating time series using indices based on the difference between calculated and measured values. Using such indices, models showing no response in time (e.g. no peak of soil ammonia mineralisation) may quantitatively perform better than models showing responses shifted in time with respect to measured data.

Confidence limits around the experimental data points, and around the results of the simulation experiment, as obtained by program sensitivity analysis (both with respect to parameters and model structure), would improve a comparison of model results and measured data (Klepper, 1989). Numerical indices and statistics may play an important role to make comparisons quantitative. For research purposes the analysis of the disagreement between data and program results may lead to new insights. Obviously, such insights and/or emerging properties can only be discovered if the program indeed fully represents the model: otherwise errors are discovered. Comparing program results with experimental data is needed, but deviations should not only induce a sound suspicion in the model, but also data should be critically (re)considered.

3.4. How to improve circumstances so that adequate models be developed?

Model documentation should comprise a scientific justification, a technical program description, and a users manual. Usually, only the scientific justification is prepared, reviewed thoroughly, and published. If, similarly to journal manuscripts, technical documentation would be prepared and reviewed, this would greatly contribute to the quality of models and modelling papers, not least because authors would go through their code once more and thus would improve it. The technical documentation should be available to colleagues on request, rather than published.

Another suggestion to develop adequate models is to develop a book, entitled for instance 'Numerical recipes in agro-ecology', that, similarly to Numerical recipes by Press et al. (1986), briefly describes commonly accepted descriptions of often used submodels. Mathematicians have understood the strength of such documentation before, given the fact that many libraries of routines are developed and used (e.g. IMSL, Nag, Linpack). One should keep in mind though, that these libraries are mostly used in an engineering setting, while the documentation proposed here should be the state of the art of quantitative agronomic science. Therefore, the refreshment rate of a book such as 'Numerical recipes in agro-ecology' should be high.

Finally, using appropriate software technologies and tools would be helpful (for further details see Section 5).

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4. Session C. Model application and development

Why are you modelling? Applications and user interaction

M.K. van Ittersum (chair)[a], C.O. Stockle (chair)[b], J.W. Jones[c], B.A. Keating[d], R.M. Matthews[e]
[a]Plant Production Systems group, Wageningen University, The Netherlands; [b]Department of Biological Systems Engineering, Washington State University, Pullman, WA, USA; [c]University of Florida, Agricultural and Biological Engineering Department, Gainesville, FL, USA; [d]CSIRO Sustainable Ecosystems/APSRU, Brisbane, Queensland, Australia; [e]Institute of Water and Environment, Cranfield University, Bedfordshire, UK

The fact that the majority of the papers for this symposium was submitted to this session shows that the application of models for various purposes is becoming increasingly important. Model use is no longer exclusively driven by researchers. Instead, there is now a broad interest in model application by government agencies and other groups, related to subjects for which the simulation models' peculiar capability of analysing agricultural systems in their various dimensions is needed. Adequately meeting this need is the challenge that cropping systems modelling is facing.

By clustering the contributions to the session, the following purposes of model application were identified:

- enhancing understanding and management of production systems;
- analysing and exploring options at farm and regional scale;
- analysis of spatial variability and interactions;
- developing summary models, for predictive purposes;
- contributing to teaching and training programs.

Further some contributions of this session addressed technical and operational aspects of applying models, and their data requirements and data management.

Related to the topic of this session, we identified a number of relevant issues that were discussed, and illustrated by oral and poster presentations.

4.1. *Target groups*

Target groups of modelling can be researchers, working at plot, cropping system, farm or regional scale, decision makers at various scales (policy makers, extension services, farmers, environmental agencies), and students or their educators. Within the research domain, descriptive and process research ('how the world works') and policy/operations and participatory action research ('how to change the world') have distinct user groups. Decision makers can be interested in short-term processes ('operational'), mid-term ('tactical') or in long-term processes ('strategic'). Educators are generally more interested in ease-of-use and ability of a model to convey a message, rather than absolute accuracy.

Target groups, therefore, will have important influence on the type of results a model should generate, the way these results are presented, and increasingly, will determine how the model is constructed and the type of components that are incorporated. If they are to use the model themselves, they may also have a say in technical aspects of the model (modelling language, interface, etc.). Further, target groups may have an important impact through their role in financing modelling efforts. Users contribute to model development by evaluating models, addressing site-specific issues, and highlighting areas of the simulation system which require development to increase both the application domains in terms of environmental conditions and the ease of use. Involvement of users is fundamental for having an impact through either learning or innovation processes. Keating and McCown (2001) and Leeuwis (1999) have recently reflected on the use of quantitative systems analysis tools in decision support, learning and innovation processes.

This raises the question of whether either the scientists ('producers') or the users ('consumers') drive model development and application. Often users, particular non-scientists, will not be primarily interested in the model, but in outcomes. Whether the outcomes are produced by some kind of quantitative model, or any other type of research is not of prime concern to them. It stresses again that modelling is a means rather than an end in itself.

4.2. *What is the evidence of application and impact?*

This question immediately triggers the question 'how to define and measure impact'. If impact stands for some kind of benefit in the understanding of systems, testing hypotheses, integrating and structuring knowledge and designing of experiments, there is ample evidence of impact. Perhaps the most evident, but often forgotten, impact is that modelling has enhanced quantitative, systems thinking in many places in the world. When it comes to evident examples of impact in agricultural practice, policy making, or land use the answer to the question of impact might be less positive (see e.g. Matthews and Stephens, 2002), at least this question is much more difficult to answer.

4.3. *How can model applications be enhanced?*

Crop models are being applied everywhere and for a broad range of issues. Their application in problem solving may be more subtle than we have recognised in the past. They contribute to a *process* of problem solving as opposed to being the only or even major tool used in many cases. Limitations to model application may relate, in random order, to technical issues, data requirements, model quality, model documentation and access to models (Sections 3 and 5). These evident limitations are complemented by a constraint which is related to the gap that may exist between how scientists model aspects of the real world and how users perceive those aspects in their own (often mental) models. Increasingly, it is recognised that the use of models should be embedded in an action learning cycle, contributing to observations and reflections of actors that may lead to planning and action. Initial successes of such a more modest and 'realistic' role for modelling have been reported (e.g. Keating and McCown, 2001).

4.4. Do we need to close the loop between users and developers?

The symposium in Florence clearly showed that the answer to this question should be 'yes'. Too many modelling efforts are fragmented and poorly co-ordinated without a proper feedback between users and developers. Often, the reason a researcher wants to use a model is not to contribute to model development, but rather to apply the model to solving a particular problem. Furthermore, how can progress be made when most financial support is aimed at problem solving as opposed to model development? Although users are interested in outcomes of model application to solve problems, only in few occasions a model can be used without any modification in its structure or parameters. The lack of feedback between the user and the developer means that all experience derived from the model application is lost. Different modelling groups around the world try to organise 'closing of the loop' in different ways (see second special issue: Brisson et al., 2003; Jones et al., 2003; Keating et al., 2003; Stöckle et al., 2003; Van Ittersum et al., 2003), with distinct consequences for availability and support of the various packages.

5. Session D. Software development and demonstration

Which software designs for evolution?

M. Donatelli[a] (chair), J. Bolte[b], F. van Evert[c], E. Wang[d]
[a]Research Institute for Industrial Crops, Bologna, Italy; [b]Department of Bioresource Engineering, Oregon State University, Corvallis, OR, USA; [c]Plant Research International, Wageningen University and Research Centre, The Netherlands; [d]APSRU, Department of Primary Industries, Toowoomba, Queensland, Australia

When modelling activity in the domain of crop/cropping systems started more than three decades ago, modellers typically developed a conceptual model, and then coded it into a programming language to perform the needed computations. Later, in many research groups, a programmer was involved, but clear limits were imposed due to both computer language legacy and the desire of the modeller to access the code directly. In the last decade, integrated software development environments and object-oriented techniques became available. It is generally agreed that the use of object-orientation, although not generalised to cropping system programs, improved the readability and reusability of code. However, even within an object paradigm, the code of most simulation models is still relatively inaccessible and reflects the developer's specific way of defining *objects*. Often, model development is still done by the modeller translating the equations of the conceptual model into code (either directly or via a programmer). Moreover, model documentation in reality is often obsolete with respect to the computer program.

When evaluating the state of the art of cropping systems models from the point of view of software design, the question session D was meant to address was: to what extent do recent advances in software engineering satisfy the needs of the modelling community, and to what extent are these advances being used in model development?

5.1. Modularity and reusability

In systems analysis, it is common to deal with the complexity of an entire system by considering it to consist of independent sub-systems. This leads naturally to consider models as consisting of submodels. Such a (conceptual) model can be implemented as a computer model that consists of a number of connected *component* models. An implementation that consists of component models has at least two major advantages. First, new models could be constructed by connecting existing component models of known quality with new component models. This has the potential to increase the speed of development. Secondly, the predictive capabilities of two different component models can be compared. Further, frequently used generic simulation, presentation and analysis functionality can be developed once and readily shared by model developers.

Despite the simplicity and intuitiveness of this concept, putting this into practice has a large impact on software design. Currently, many research groups feel that they have significantly improved reusability because they have changed the code of their prototypes by implementing structured programming. While this can substantially improve code readability, structured programming methods have done little to improve reusability. A noticeable step in the area of conceptualising modularity in crop models is presented by Wang et al. (2003). With respect to the software aspects, the key concept for reusability is the use of *interfaces*, i.e. the set of operations that is possible on a component model. An interface standardises communication across models, which facilitates reusability. At the same time, the language code for algorithms is not critical given the *wrapping* provided by the interface, thus eliminating or minimising the problem of code legacy. Modularity and reusability can be implemented using the proper software technique, but of course model conceptualisation remains critical.

5.2. Model conceptualization

While reusability is a key issue for efficient use of resources and model comparison, there is also a need for complete transparency, reproducibility and verification of models as components of scientific argumentation (Muetzelfeldt and Massheder, 2003). Transparency (the ability of a model to be a self-documenting construct) is hardly achievable if model development consists of coding equations and producing corresponding model documentation through a separate process. Forrester diagrams (Forrester, 1961), universal modelling language, and other visual notations can be used to describe simulation systems. During session D two papers where presented showing examples of applications of the formal descriptions of models via visual tools (Papajorgji et al., 2001; Muetzelfeldt et al., 2001). These visual environment software tools allow translating the conceptual model into code. This is very important as it allows the modeller to concentrate on the simulation approach, which is described via a graphical language, rather than forcing the modeller to write code, which will necessarily include dependencies with the functioning of the whole simulation system. The use of visual modelling tools, which allow a formal description of models, is by definition cross-language and cross-platform because they provide a standard description of the model that can be easily and automatically translated into different computer languages. Finally, the visual approach allows development of models/simulation systems that are auto-documented. However, there is as yet no software that allows frequent and flexible switching between textual and graphical representations of a model.

5.3. Modelling frameworks

Three major parts of the code in cropping systems models are usually prototype specific, resource intensive, and prevent transferability: (1) data input/output (I/O) procedures (e.g. input/output data handling, file management); (2) common services (e.g. state variables integrator, events handler); and (3) graphical user interfaces. Modelling frameworks can play a key role to address these issues. First, the framework allows segregating the application-specific parts of simulations from the code employed to accomplish common tasks, thus greatly enhancing code reuse (Hillyer et al., 2003). Second, by defining the elements of the framework that actually contain the model implementation and how those elements are used, a designer can be presented with a clear path from conceptual model to simulation (Hillyer et al., 2003). Furthermore, providing common services allows concentration of resources on development of simulation components.

The use of a model framework does not imply that the modeller must continue the traditional procedure of translating equations into code. Visual tools can be developed and integrated into the modelling environment in order to match ease of use in model development to the creation of highly efficient code.

5.4. What design for future development?

Rather than being a technicality, limitations in approaches to software design have been a major reason for the lack of innovation in crop/cropping systems models. Major issues relevant to agro-ecological model development listed by Van Kraalingen, (1995) regarding simulation model development, and by Holzworth et al. (2001) regarding software engineering principles, have had a very limited impact on currently available cropping systems models. It is time to define verifiable quality standards that must be applied in order to accept model use in either the scientific or application domain.

There are several options for an efficient software design for future development, most of which have been under-utilised by the cropping systems modelling community. The software techniques used in development of agro-ecological models lie far behind the level reached in many other areas where modelling plays an important role. The key elements needed to achieve an efficient software design can be summarised as:

- modularity and reusability, implemented via interfaces and a standard, flexible communication protocol;
- use of model frameworks to provide common services;
- conceptualisation of simulation systems and submodels using a formalised description, rather than writing code;
- make documentation as an auto-generating feature of the system;
- development of benchmarks for model testing and version comparison.

Integration between software engineers and modellers is needed to achieve effective, domain specific software design and model development. As long as software design does not allow modellers to concentrate almost exclusively on process simulation, model development will not be able to integrate effectively with, and make most effective use of, research.

6. Preface to two special issues

Two special issues of the European Journal of Agronomy reflect the contents of the symposium, and even add to it in some aspects. The first issue ‘Process simulation and application of cropping system models’ (guest-edited by M. Donatelli, M. Bindi, J.R. Porter and M.K. van Ittersum: European Journal of Agronomy 18, issues 1–2, 2002) publishes ten full papers based on contributions to the symposium. The first paper (Hammer et al.) presents a vision on where to next with crop modelling. The papers by Rizzalli et al. and Tei et al. present the development of a crop model for garlic and work needed for the parameterisation of nitrogen-limited modules for tomato models, respectively; two examples of what could be classified as typical crop growth modelling papers. The next four papers all aim at some kind of evaluation and synthesis of different approaches. Tubiello and Ewert evaluate various approaches to modelling consequences of elevated CO_2 concentrations, Gijsman et al. attempt to help the reader through the swamp of many approaches for estimating soil water retention parameters, Gabrielle et al. investigate the coupling of four different modules for soil organic matter and nitrogen decomposition to a common crop growth model, and Wang et al. describe the development of a generic crop template. The first special issue is completed with three papers applying cropping system models, i.e. Batchelor et al. for purposes of analysing spatial variation within fields (precision farming), Keating et al. to evaluate various cropping systems in their water leakage, with both a comprehensive and a summary-type of model, and Huth et al. to evaluate agro-forestry systems.

The second special issue ‘Modelling cropping systems: science, software and applications’ (guest edited by M.K. van Ittersum and M. Donatelli—European Journal of Agronomy, this issue) presents overview papers on five of the world’s major systems for modelling crops and cropping systems, ordered more or less according to their age, i.e. Wageningen models, DSSAT, APSIM, CropSyst and STICS. These papers are not explicitly based on contributions to the symposium, though the five groups were all well represented in Florence. Since no recent papers describing these systems in scientific journals are available, the groups were invited to write these overview papers, using similar outlines. The next two papers (Hillyer et al.; Muetzelfeldt and Massheder) describe technical frameworks that show recent software developments which can be of great help in developing integrated frameworks for crop modelling, and the development of transparent modular approaches. The final 6 papers of the second special issue are short communications describing modelling environments or software packages relevant to modelling crops and cropping systems, both for researchers, users and students.

The papers give an overview of what has been achieved so far, and they point at the questions that modellers of cropping systems face in the next decade. They also show the prospects and tools that can further increase the relevance of cropping systems modelling and its application to the benefit of developing sustainable agricultural production systems. We trust that these special issues will not only be of interest to those that have attended the symposium, but also to those around the globe, be it agro-ecologists, agronomists or other scientists, students or stakeholders, interested in, working with or making use of modelling cropping systems.

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M.K. van Ittersum
Plant Production Systems Group,
Wageningen University,
P.O. Box 430,
6700 AK Wageningen,
The Netherlands

M. Donatelli
Research Institute for Industrial Crops,
Via di Conticella, 133,
40128 Bologna,
Italy