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Ten iterative steps in development and evaluation of environmental models

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Abstract

Models are increasingly being relied upon to inform and support natural resource management. They are incorporating an ever broader range of disciplines and now often confront people without strong quantitative or model-building backgrounds. These trends imply a need for wider awareness of what constitutes good model-development practice, including reporting of models to users and sceptical review of models by users. To this end the paper outlines ten basic steps of good, disciplined model practice. The aim is to develop purposeful, credible models from data and prior knowledge, in consort with end-users, with every stage open to critical review and revision. Best practice entails identifying clearly the clients and objectives of the modelling exercise; documenting the nature (quantity, quality, limitations) of the data used to construct and test the model; providing a strong rationale for the choice of model family and features (encompassing review of alternative approaches); justifying the techniques used to calibrate the model; serious analysis, testing and discussion of model performance; and making a resultant statement of model assumptions, utility, accuracy, limitations, and scope for improvement. In natural resource management applications, these steps will be a learning process, even a partnership, between model developers, clients and other interested parties.

Keywords: Model testing; Verification; Uncertainty; Sensitivity; Integrated assessment; System identification

1. Motivation

The pursuit of good practice in model development and application deserves thorough and sustained attention, whatever the field. Good practice increases the credibility and impact of the information and insight that modelling aims to generate. It is crucial for model acceptance and is a necessity for long-term, systematic accrual of a good knowledge base for both science and decision-making. The complexity and uncertainty inherent in management for better sustainability outcomes make the pursuit of good practice especially important, in spite of limited time and resources. Natural resource management confronts a complex set of issues, usually with environmental, social and economic trade-offs. These trade-offs are characterised by interactions at many scales and often by scarcity of good observed data. Thus natural resource managers commonly have to trade uncertain outcomes to achieve equitable results for various social groups, across spatial and temporal scales and across disciplinary boundaries. This must be achieved on the basis of information that varies in relevance, completeness and quality.

The complexity of these situations has led to model-based approaches for examining their components and interactions, and for predicting management outcomes. There is wide agreement on the potential of models for revealing the implications of assumptions, estimating the impact of interactions, changes and uncertainties on outcomes, and enhancing communication between researchers from different backgrounds and between researchers and the broader community.

Managers and interest groups can also potentially benefit from use of a model to define the scope of a problem, to

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make assumptions explicit, to examine what is known and what is not, and to explore possible outcomes beyond the obvious ones. If models are accessible enough, they can act as a medium for wider participation in environmental management. However, the pressing need to use models in managing

Footnote for first page of position paper:

Position papers aim to synthesise some key aspect of the knowledge platform for environmental modelling and software issues. The review process is twofold – a normal external review process followed by extensive review by EMS Board members. See the Editorial in this issue.

Complex situations, rather than in sharply defined areas of research, has resulted in people with little modelling or quantitative background having to rely on models, while not being in a position to judge their quality or appropriateness. Caminiti (2004) provides a resource manager's perspective on the difficulties of choosing the best modelling approach for catchment management, concluding that "[m]odellers can help by trying to understand the needs and expectations of the resource manager, who may not have the technical knowledge or language to express them." Managers may also not initially understand their own needs fully, so modelling must be an iterative learning process between modeller and manager.

The uses of models by managers and interest groups, as well as by modellers, bring dangers. It is easy for a poorly informed non-modeller to remain unaware of limitations, uncertainties, omissions and subjective choices in models. The risk is then that too much is read into the outputs and/or predictions of the model. There is also a danger that a model is used for purposes different from those intended, making invalid conclusions very likely. Taking a longer-term perspective, such inadvertent abuses detract from and distort the understanding on which science and decision-making are built.

The only way to mitigate these risks is to generate wider awareness of what the whole modelling process entails, what choices are made, what constitutes good practice for testing and applying models, how the results of using models should be viewed, and what sorts of questions users should be asking of modellers. This amounts to specifying good model practice, in terms of development, reporting and critical review of models.

As a move in that direction, this paper outlines ten steps in model development, then discusses minimum standards for model development and reporting. The wide range of model types and potential applications makes such an enterprise prone to both over-generalisation and failure to cover all cases. So the intention is to name the main steps and give examples of what each includes, without attempting the impossible task of compiling a comprehensive checklist or map of the model-development process. Such checklists have been developed within certain modelling communities where particular paradigms are dominant. Thus the Good Modelling Practice Handbook (STOWA/RIZA, 1999), financed by the Dutch government and executed by Wageningen University, has a well developed checklist for deterministic, numerical models. The guidelines for modelling groundwater flow developed by the Murray-Darling Basin Commission (2000) in Australia provide another example. Our purpose, by contrast, is to point to considerations and practices that apply in a broad range of natural resource modelling situations.

It is hoped that this paper will prompt modellers to codify their practices and to be more creative in their examination of alternatives and rigorous in their model testing. It is intended to provide a synoptic view for model builders and model users, applying to both integrated models and models within distinct disciplines. It does not deal with the surrounding issue of the appropriate development and use of environmental decision support systems (e.g. Denzer, 2005), which in addition involve issues of user interfacing, software usability and software and data integration. The paper discusses good practice in construction, testing and use of models, not in their imbedding and use in decision support systems or with software interfaces more widely.

As already indicated, the idea of guidelines for good model practice is not new. Parker et al. (2002) call for the development of guidelines for situations where formal analysis and testing of a model may be difficult or unfeasible. They state that "the essential, contemporary questions one would like to have answered when seeking to evaluate a model (are):

i) Has the model been constructed of approved materials i.e., approved constituent hypotheses (in scientific terms)?
ii) Does its behaviour approximate well that observed in respect of the real thing?
iii) Does it work i.e. does it fulfil its designated task, or serve its intended purpose?"

Risbey et al. (1996) call for the establishment of quality-control measures in the development of Integrated Assessment (IA) models for climate change, and suggest several features that must be considered:

- a clear statement of assumptions and their implications;
- a review of 'anchored' or commonly accepted results and the assumptions that created them;
- transparent testing and reporting of the adequacy of the whole model, not only each of the component parts;
- inclusion of the broadest possible range of diverse perspectives in IA development;
- supply of instructions to model end-users on the appropriate and inappropriate use of results and insights from the analysis;
- 'A place for dirty laundry', that is, for open discussion of problems experienced in constructing complex integrative modelling, in order for solutions to these problems to be found, and to facilitate the appropriate level of trust in model results.

Ravetz (1997), considering integrated models, argues for validation (or evaluation) of the process of development rather than the product, stating that in such circumstances "the inherently more difficult path of testing of the process may actually be more practical". Ravetz finds that in general "the quality of a model is assured only by the quality of its production".

However, he does not define the essential components or steps in model development that would make up such a quality-assurance process, nor does he discuss how far the quality of production can be assessed without assessing the quality of the product.

Caminiti (2004) outlines a number of potential pitfalls in using models for management, and proposes steps that resource managers should take to avoid them.

Refsgaard et al. (2005) address the issue of quality assurance (QA), defined as protocols and guidelines to support the proper application of models. They argue that "Model credibility can be enhanced by a proper modeller-manager dialogue, rigorous validation tests against independent data, uncertainty assessments, and peer reviews of a model at various stages throughout its development."

In promoting responsible and effective use of model information in policy processes, Van der Sluijs et al. (2005) discuss four case-study experiences with the NUSAP system for uncertainty assessment. This system, due to Funtowicz and Ravetz (1990), offers analysis and diagnosis of uncertainty in the knowledge base of complex policy problems. Van der Sluijs et al. (2005) show that extending the scheme beyond mainstream technical methods of sensitivity and uncertainty analysis, by complementing it with qualitative approaches, further promotes reflection and collective learning. Thus they cover societal aspects such as differences in framing of the problem, inadequacy of institutional arrangements at the science-policy interface, and controversy.

These authors argue that good practice in the development of integrated models is made all the more necessary by the inherent difficulties in validating them. As implied in the opening paragraph, many disciplinary modelling studies lack elements of good model practice, such as a clear statement of modelling objectives, adequate setting out of model assumptions and their implications, and reporting of model results, including validation/evaluation. Cross-disciplinary models for influencing management should be tested against additional criteria such as fitness for purpose, flexibility to respond to changing management needs, and transparency so that stakeholders can see how the results were derived.

2. Improving the modelling process

2.1. Introduction

Broad areas where better modelling practice can improve models and their adoption are suggested below, before more detailed discussion of ten steps in model development.

Wider and more strategic application of good models, comparison of models and associated long-term data acquisition can assist not only in exploiting existing knowledge but also in accruing new knowledge. An example is the current Prediction in Ungauged Basins program of the International Association of Hydrological Sciences. It has several groups, one the Top-Down Working Group (http://www.stars.net.au/tdwg/). The groups are tackling questions of how to predict streamflow in ungauged catchments through systematic studies, typically involving comparison of traditional and novel models and dataset benchmarking across a range of hydroclimatologies. The Top-Down Working Group expects to improve understanding of the drivers of catchment processes and how they relate to fluxes from river basins. Its success will depend on attention to the areas outlined below.

2.2. Proper definition of scope and objectives of the model

In making a case for modelling to help managers respond to a problem in natural resources, it is all too easy:

- to extend the scope beyond what is needed to answer the questions at hand;
- to promise more than can be delivered in the time available;
- to ignore or underestimate the difficulties and the limitations in data and techniques;
- to oversimplify or overelaborate;
- to push a particular approach not well suited to the job;
- to rely too much on existing, familiar but less-than-ideal models, and conversely;
- to overlook existing knowledge and previous experience;
- to take too little note of the need for consultation and cooperation;
- to commit to a time scale preventing unforeseen factors from being adequately dealt with, and, most crucially;
- to obfuscate the objectives, knowingly or inadvertently.

How often does one see objectives explicitly stated *and iterated upon*? Refinement of an objective can lead to a simpler task, as some factors are found to be unimportant, others critical, and the available information becomes clearer. Assessment of uncertainty plays a crucial role in such refinement; better a useful answer to a simple question than too uncertain an answer to a more ambitious question.

2.3. Stakeholder participation in model development

Stakeholders comprise all those with an interest. For natural resources, this is especially the managers and the various sectoral interests. Stakeholder participation is a key requirement of good model development, particularly when models are to address management questions. Aside from equity and justice, there are two main reasons for increased stakeholder participation in model development. The first is to improve the modeller's understanding, allowing a broader and more balanced view of the management issue to be incorporated in the model. The second is to improve adoption of results from the assessment, increasing the likelihood of better outcomes, as model development becomes an opportunity for stakeholders to learn about interactions in their system and likely consequences of their decisions. Both reasons work iteratively. That is, continued involvement is necessary because neither the modeller nor the manager usually has a clear and comprehensive idea at the outset of what the model must do.

Stakeholder participation in the past has often been limited to researchers wishing to exploit the results of the modelling exercise. A better approach, increasingly employed, is to involve all stakeholders throughout model development in a partnership, actively seeking their feedback on assumptions and issues and exploiting the model results through feedback and agreed adoption. This approach is expensive in effort, time and resources, but the aim of modelling is often to achieve management change, and the learning process for modellers, managers and other stakeholders inherent in this approach is essential to achieving change. Examples of such participation in model development can be found in Fath and Beck (2005), Hare et al. (2003) and Letcher and Jakeman (2003). Beck (2005) "examines the implications of the ongoing shift – from the technocracy of the past century to the democracy of stakeholder participation in the present century – for the more widespread use of information and technologies in managing water quality in urban environments." An excellent overview of participation as part of integrated assessment can be found in Mostert (in press).

2.4. Conceptualising the system

Consideration and justification of options in defining the system warrant attention by modellers and their clients. What to include and what not to incorporate in a modelling activity should be addressed explicitly at the outset and iteratively revisited as far as resources allow. The system being modelled should be defined clearly, including its boundaries (e.g. physical, socioeconomic and institutional). Boundary conditions can then be modelled as constraints or as input scenarios, whose values can be perturbed in line with stipulated assumptions.

2.5. Embracing alternative model families and structures

Comparisons between alterative model families and structures are sometimes advocated (as above), but seldom performed systematically against specified criteria or, indeed, at all in environmental modelling. Failure to carry out comparisons is understandable, given that most modellers have strong preferences for particular model structures and model-development approaches. Such preferences may be built on experience and constrained by resource limitations or lack of open-mindedness. In an ideal world, a modelling project would be let out to two or more groups to encourage rigorous comparison. In the real world, with limited resources, sponsors of modelling could have a strong influence by demanding comparisons, if they took the view that a limited but thorough exercise is preferable to a more ambitious but less well tested one.

A growing risk is that the wider community, decision-makers and politicians are effectively disfranchised by inability to weigh up conclusions drawn from models. Inadequate reporting and absence of discussion of alternatives can result in unsystematic, specialised representation of accrued knowledge, not open to challenge. This becomes profoundly unsatisfactory when model-based conclusions are susceptible to gross error through lack of good practice. In some areas where there is a consensus on modelling issues but not solutions, a remedy may be to seek more collaborative and strategic science, funded to bring groups together internationally to execute comparative studies. The EU Research Frameworks have such aims among others and are beginning to take a wider perspective outside Europe, but there is a need for more flexible, rapidly responding, heterogeneous, informal yet long-term arrangements. Long-term, consistent collaboration is needed across a range of modelling communities, to generate systematic knowledge representation and testing, gradually developing a widely understood and accepted methodological platform on which to build and test models.

2.6. More comprehensive testing of models

Environmental models can seldom be fully analysed, if only because of the heterogeneity of their data and the range of factors influencing usefulness of their outputs. In the case of groundwater models, Konikow and Bredehoeft (1992) argue from a philosophical and practical viewpoint that the strong term "validation" has no place in hydrology. They indicate that Hawking (1988) has generalised this further to state that "Any physical theory is always provisional, in the sense that it is only a hypothesis: you can never prove it." Oreskes et al. (1994) examine the philosophical basis of the terms "verification" and "validation" as applied to models. What typically passes for these terms is at best confirmation to some degree. The two terms imply a stark choice between acceptance and rejection. On the contrary we recognise that model performance may be assessed against many criteria, and that often no sharp acceptance threshold exists. We urge discussion of performance, recommending that a wide range of performance indicators be examined. The problem-dependent indicators selected may include:

- satisfactory reproduction of observed behaviour;
- high enough confidence in estimates of model variables and parameters, taking into account the sensitivity of the outputs to all the parameters jointly, as well as the parameter uncertainties;
- plausibility of the model properties, e.g. values which conform with experience for biophysical and socioeconomic parameters and means or extremes of associated variables;
- absence of correlation between model residuals (output errors) and observed inputs, since correlation indicates unmodelled input-output behaviour;
- time- and space-invariance of parameter estimates, since variation indicates poorly or incompletely specified parameters (unmodelled behaviour again);
- satisfactory properties of the residuals, such as absence of significant structure over time and space, e.g. constant mean and variance;
- consistency of the model in cross-validation against different sections of the input-output records (Janssen et al.,

1988) and perhaps also against perturbations of the data typical of their errors;
- along with these technical aspects, a range of model characteristics important to managers and stakeholders, including transparency and flexibility.

One could take this a step further by not only performing and reporting on model checks, but also asking for independent model auditing to provide safeguards to end-users.

2.7. Detection and reduction of overfitting

Model structures with too many parameters are still endemic. Models with too many degrees of freedom incur serious risks. Among them are: fitting to inconsistent or irrelevant "noise" components of records; severely diminished predictive power; ill defined, near-redundant parameter combinations; and obscuring of significant behaviour by the spurious variation allowed by too much freedom. Even so, model testing for redundancies and possible model reduction are seldom reported. Data paucity should limit the model complexity. For example, in modelling of flow and transport for prediction, spatial data on landscape attributes may be useful to structure and discretise a model in fine detail, but detail is unwarranted if the flux measurements available for model calibration cannot support it (Jakeman and Hornberger, 1993). A related sin is the use of a favourite model even when it is overparameterized for the data available. Indeed there are instances in the literature of simple models with well identified parameters working better than complex models where less formal attention is paid to the parameters. One is Marsili-Libelli and Checchi (2005). They observe that "The current trend in horizontal subsurface constructed wetlands (HSSCW) modelling advocates structures of increasing complexity, which however have produced a limited improvement in the understanding of their internal functioning or in the reliable estimation of their parameters." Their proposed use of simple model structures in combination with robust identification algorithms deserves attention in a wider domain than HSSCW modelling.

3. Ten steps

Whatever the type of modelling problem, certain common steps must be considered if the goals are credible results and knowledge acquisition, for the immediate purpose of the exercise and for the wider community and the longer term. Major steps have been elucidated, for example, by Jorgensen and Bendoricchio (2001) for ecological modelling, Seppelt (2003) for landscape ecology, Grafton et al. (2004) for economic-environmental systems and Wainwright and Mulligan (2004) for environmental modelling. Young (1993) summarizes a detailed set of steps for a "typical statistical environmental modelling procedure" and comments that it is an interpretation of the scientific method from the Popper viewpoint. The guidance offered by these authors partly complements and partly overlaps ours. We are trying to be more generic and to suggest guidelines for a wide range of model types. It would be futile to try to categorise families of models comprehensively, but the list below serves to illustrate the breadth of choice. In the main we also avoid reference to real-life examples. Model families and their features include:

- empirical, data-based, statistical models, with structures chosen primarily for their versatility and assuming little in advance, e.g. data-mined clusters, parametric or non-parametric time series models, regressions and their generalisations such as autoregressive moving-average exogenous models, power laws, neural nets;
- stochastic, general-form but highly structured models which can incorporate prior knowledge, e.g. state-space models and hidden Markov models;
- specific theory-based or process-based models (often termed deterministic), as often used in environmental physics and economics, e.g. specific types of partial or ordinary differential or difference equations;
- conceptual models based on assumed structural similarities to the system, e.g. Bayesian (decision) networks, compartmental models, cellular automata;
- agent-based models allowing locally structured emergent behaviour, as distinct from models representing regular behaviour that is averaged or summed over large parts of the system;
- rule-based models, e.g. expert systems, decision trees;
- a spectrum of models which represent dynamics (time-spread responses to the inputs at any given instant) in differing degrees of detail. This spectrum spans instantaneous (static, non-dynamical), discrete-event and discrete-state models (e.g. Petri nets, Markov transition matrices), lumped dynamical (finite-state-dimensional, ordinary differential equation), distributed (partial differntial equation) and delay-differential infinite-state-dimensional models;
- a corresponding spectrum of spatial treatments, comprising non-spatial, 'region-based' or 'polygon-based' spatial, and more finely (in principle continuously) spatially distributed models (e.g. finite-element/grid-based discretisations of partial differential equations).

Many authors also find it useful to distinguish between white box (theory-based), black box (empirical) and grey box (theory-influenced empirical) models (e.g. Seppelt, 2003). The steps we shall delineate are appropriate whether the exercise employs traditional models, e.g. the dynamical-statistical families of models considered by Ljung (1999), Norton (1986), Söderström and Stoica (1989), and Young (1984); the empirical, deterministic or conceptual families covered by Jakeman et al. (1993); more recent artificial-intelligence or "knowledge-based" model types (e.g. Davis, 1995; Forsyth, 1984; Kidd, 1987; Schmoldt and Rauscher, 1996); or a mixture. Most of the essential features of development practice outlined in this section are shared by all these types of model. In addition we broaden the context to include the specification of objectives, choice of approach for finding model structures, involvement of interest groups, and choice of parameter estimation methods and algorithms. Although examples will be given, the focus throughout is mainly on what questions must be addressed, not what alternatives exist.

The steps sketched in Fig. 1 and listed below are largely iterative, involving trial and error. If there is pressure to use an already developed model for all or part of the exercise, attention to all steps remains warranted. That is, the steps proposed are not just of relevance for developing a new model. Depending on the purpose, some steps may involve end-users as well as modellers. The steps are not always clearly separable. For instance, it is a matter of taste where the line is drawn between model-structure selection and parameter estimation, as model structures are partly defined by structural parameters.

3.1. Definition of the purposes for modelling

It is a truism that the reasons for modelling should have a large influence on the selecting of a model family or families (see Section 2.5) to represent the system, and on the nature and level of diagnostic checking and model evaluation. However, it is not necessarily easy to be clear about what the purposes are. Different stakeholders will have different degrees of interest in the possible purposes of a single model. For example, a resource manager is likely to be most concerned with prediction, while a model developer or scientific user may place higher stress on the ability of the model to show what processes dominate behaviour of the system. That said, better understanding is valuable for all parties as part of defining the problem and possible solutions, and as a means of assessing how much trust to place in the model. It is important to recognize that some purposes, particularly increased understanding of the system and data, may be realised well even if the final model is poor in many respects. An inaccurate model may still throw light on how an environmental system works.

Purposes include:

- gaining a better qualitative understanding of the system (by means including social learning by interest groups);
- knowledge elicitation and review;
- data assessment, discovering coverage, limitations, inconsistencies and gaps;
- concise summarising of data: data reduction;
- providing a focus for discussion of a problem;
- hypothesis generation and testing;
- prediction, both extrapolation from the past and ‘‘what if’’ exploration;
- control-system design: monitoring, diagnosis, decision-making and action-taking (in an environmental context, adaptive management);
- short-term forecasting (worth distinguishing from longer-term prediction, as it usually has a much narrower focus);
- interpolation: estimating variables which cannot be measured directly (state estimation), filling gaps in data;
- providing guidance for management and decision-making.

These motives are not mutually exclusive, of course, but the modeller has to establish the purposes and priorities within the

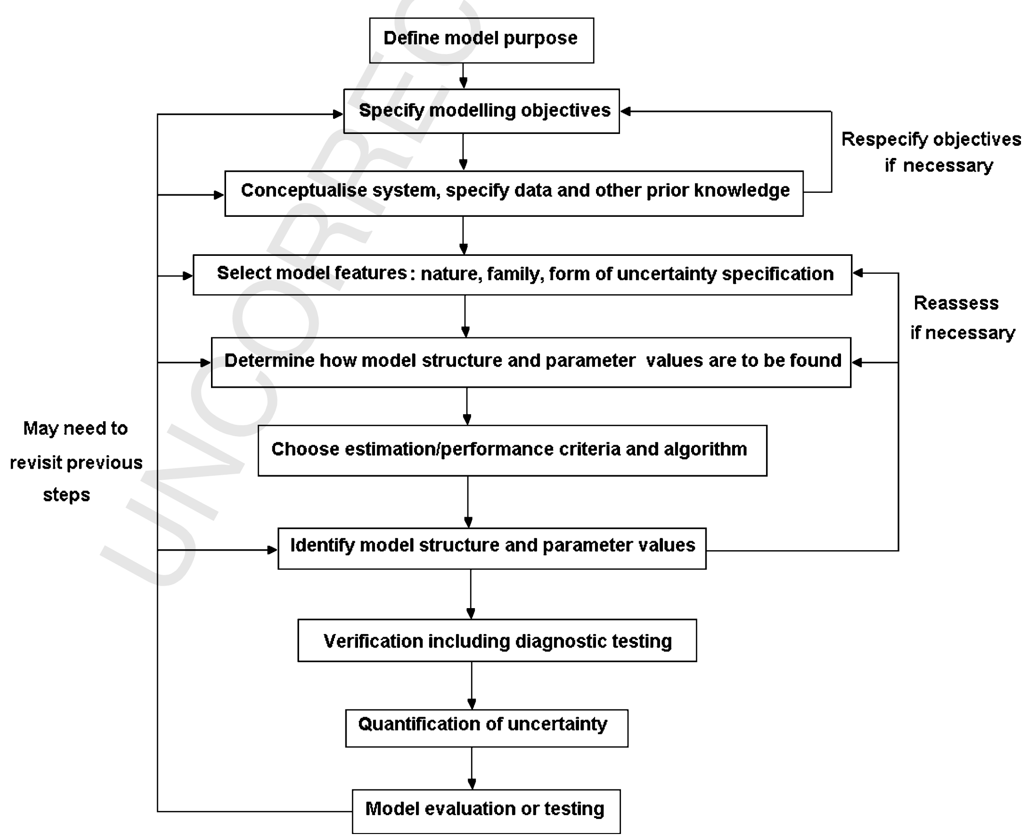

Fig. 1. Iterative relationship between model building steps.

list, because of their influence on the choices to be made at later stages. For example, economy in the degrees of freedom of a prediction model (''parsimony'') is important if the model is to register the consistent behaviour observed in the data but not the ephemeral, inconsistent ''noise.'' Experience confirms that it is often counterproductive to include much detail in a prediction model for a restricted purpose (Jakeman and Hornberger, 1993). Conversely, a model designed to increase insight into the processes which determine the system's overall behaviour has to be complex enough to mimic those processes, even if only very approximately. A model intended for knowledge elicitation or hypothesis generation may have a provisional structure too elaborate to be validated by the data, but may be simplified when the knowledge or hypotheses have been tested. Reichert and Omlin (1997) point out possible difficulties in prediction using a parsimonious model with too little flexibility to accommodate changes in perception of which processes are significant. They discuss how to identify and employ non-parsimonious models for prediction. For the modelling of wastewater treatment plants, Gernaey et al. (2004) give some excellent examples of how model purpose influences model selection, data selection and model calibration.

It is worth stressing that improvement of understanding of the system is almost always a purpose of modelling, even when the users say otherwise. The quality of management decisions rests ultimately on how well the system is understood, not merely on the quality of model predictions: insight must, on average, improve decisions. Moreover, increased understanding is often the useful outcome of a modelling exercise which is, by its stated criteria, a failure.

3.2. Specification of the modelling context: scope and resources

This second step identifies:

- the specific questions and issues that the model is to address;
- the interest groups, including the clients or end-users of the model;
- the outputs required;
- the forcing variables (drivers);
- the accuracy expected or hoped for;
- temporal and spatial scope, scale and resolution (but see also Section 3.3);
- the time frame to complete the model as fixed, for example, by when it must be ready to help a decision;
- the effort and resources available for modelling and operating the model, and;
- flexibility; for example, can the model be quickly reconfigured to explore a new scenario proposed by a management group?

A crucial step here is to decide the extent of the model, i.e. where the boundary of the modelled system is. Everything outside and not crossing the boundary is ignored. Everything crossing the boundary is treated as external forcing (known or unknown) or as outputs (observed or not). The choice of a boundary is closely tied in with the choice of how far to aggregate the behaviour inside it. Classical thermodynamics gives an object lesson in the benefits of choosing the boundary and degree of aggregation well, so as to discover simple relations between a small number of aggregated variables (e.g. energy) crossing the boundary, without having to describe processes inside the boundary in detail. In environmental management, deciding on the boundary and degree of aggregation is a critical but very difficult step. It can usually only be learnt through trial and error, since managers and stakeholders usually do not initially know the boundaries of what should be modelled.

Flexibility can be a major practical issue in matching the scope of the model to resources. For example, the time taken to introduce a new management practice proposed by an interest group might be an issue, given that, for instance, data/GIS layers need to be redrawn. A further concern is the resources to operate the model. In this example, can it be operated by people without GIS training and equipment? More generally, what specialist knowledge does a user need in order to modify a model parameter?

3.3. Conceptualisation of the system, specification of data and other prior knowledge

Conceptualisation refers to basic premises about the working of the system being modelled. It might employ aids to thinking such as an influence diagram, linguistic model, block diagram or bond graph (Gawthrop and Smith, 1996; Wellstead, 1979), showing how model drivers are linked to internal (state) variables and outputs (observed responses). Initially the conceptualisation may be rudimentary, with details postponed until the results of knowledge elicitation and data analysis can be exploited. A tentative initial conceptualisation and a visualisation such as a block diagram may be a great help in showing what else must be found out about the system.

The conceptualisation step is important even if a model is not designed from scratch because time and money (as well as the clients' beliefs) restrict one to using a 'canned' model. Conceptualisation exposes the weaknesses of the canned approach and perhaps ways to mitigate them.

This third step defines the data, prior knowledge and assumptions about processes. The procedure is mainly qualitative to start with, asking what is known of the processes, what records, instrumentation and monitoring are available, and how far they are compatible with the physical and temporal scope dictated by the purposes and objectives. However, it becomes quantitative as soon as we have to decide what to include and what can be simplified or neglected. What variables are to be included, in how much detail? Once the outputs are selected, a rough assessment is needed of which drivers they are sensitive to and what internal processes influence the relations between the drivers and outputs; this will usually be partly a quantitative assessment.

The degree of aggregation and the spatio-temporal resolution (intervals and accuracy) of the outputs also have to be chosen but, as for all these decisions, the choices may have to be revised as experience grows. The time-step and the bounds of what is to be modelled may have to be modified part way through an application, perhaps more than once. This is not trivial. Few models are flexible enough to respond to these evolving needs, which are commonly passed off by modellers as due to the client "not thinking their problem through properly at the beginning."

The first part of this step is just to state what degree of detail is needed in the outputs. However, the next step is to follow up the implications: the internal resolution of the model must be sufficient to produce outputs at the required resolution, and the time and spatial intervals throughout the model must be compatible with the range of rates of change of the variables. The only way to ensure that these requirements are met is by a careful quantitative assessment. Such assessment takes considerable effort and insight into the processes operating in the system, so it is often given too little attention. Too often sampling intervals in time and space are chosen by guesswork or simply because data are available at those intervals. Ill-chosen intervals can destroy the validity of the model, but once recognized can be amended as part of the learning process.

"Prior knowledge" can be genuinely known in advance, found from experiments or analyses performed as part of model development, or assumed, with reservations, on the basis of experience. It includes observational data and their properties (including error characteristics), structural information (e.g. coupling or independence, additivity of effects or interaction, existence of feedbacks), the nature of processes (e.g. stationarity, correlations, directionality of flows, conservation laws, switching between modes), the extent and nature of spatio-temporal forcing, and parameter values and their uncertainties. Quantitative information on uncertain parameters and errors may consist of point estimates and variances or covariances, bounds (ranges) or, if you are lucky, probability distributions.

For some environmental systems one has the luxury of optimal experimental design where inputs (such as to a bioreactor) can be manipulated to enhance the identifiability of a model (e.g. Versyck et al., 1994; Walter and Pronzato, 1997). For most systems, however, we must at any given time accept the data that are available. On the other hand, modellers can play a more proactive role in designing future data collection exercises. Monitoring efforts in the global change community are amongst the most striking.

3.4. Selection of model features and families

Any modelling approach requires selection of model features, which must conform with the system and data specification arrived at above. Major features such as the types of variables covered and the nature of their treatment (e.g. white/black/grey box, lumped/distributed, linear/non-linear, stochastic/deterministic) place the model in a particular family or families. Model structure specifies the links between system components and processes. Structural features include the functional form of interactions, data structures or measures used to specify links, spatial and temporal scales of processes and their interactions, and bin sizes for AI techniques such as data-mining. Features help to sharpen the conceptualisation and determine what model synthesis and calibration techniques are available. In simpler models, a common set of features will apply throughout, but a more complex integrated model may well be a hybrid, with the feature set varying from one part to another. For example, a deterministic or statistical climate-prediction model might interface with a non-statistical but empirical rainfall-runoff model, then with an irrigation model consisting of predetermined rules.

Families and features often overlap, and in some cases families can even be transformed into each other. For instance linear, constant-coefficient, ordinary differential equations can be transformed into, or from, Laplace or Fourier transfer functions. The choice depends on the purpose, objectives, prior knowledge and convenience.

For prediction and/or management, a key question is what the subjects of predictive or management interest are. For example is a qualitative idea of behaviour (e.g. direction of change) required, or a rough indication of the extent of a response, an extreme value, a trend, a long-term mean, a probability distribution, a spatial pattern, a time series, the frequency or location of an event? These questions aren't asked thoroughly enough at the beginning of model projects. That said, the initial answers can easily change as the project develops, especially when managers are involved, emphasizing again the need for iteration.

The selection of model family should also depend on the level (quantity and quality) of prior information specified in step 3.3. It must take account of what can be determined and how far, i.e. to which accessible and inaccessible variables the model outputs are sensitive, what aspects of their behaviour must be considered, and the associated spatial dimensions and sampling intervals in space and time.

At this stage a first judgement has to be made of how prominent uncertainty is likely to be. It will help to set reasonable expectations of capability (e.g. predictive power), and to decide whether and how randomness should be included in the model formulation. It may include an estimate of how far past observed behaviour can be extrapolated into the future or into changed circumstances.

Selection of model features and families should be flexible, prepared for revision according to evaluation of the reasonableness of initial guesses. However, in practice it is usually difficult to change fundamental features of a model beyond quite an early stage, for understandable but regrettable human reasons like unwillingness to admit a poor choice or abandon something into which much effort has already gone. A preference for a particular model, due to familiarity, established acceptance by the technical community or availability of tools for it, often impedes change.

The difficulty is exacerbated by uncertainty and changes of mind about the factors which define model features and family (part of the learning process). The problem is that expenditure and commitment to models based on the initial judgements are usually too powerful to allow any significant changes to be made. The result may well be an inappropriate model. An initial exploration with a crude, cheap, disposable model would often be a better start, so long as there is enough time and flexibility of mind to allow later choices.

Model structure covers the degree of detail permitted. It may include the choice of spatial units (e.g. hydrological response units or grid cells) and corresponding variables (e.g. points where flows and precipitation are represented), the order of a differential equation representing a process, and whether or not non-linearity or time variation is included in a relation. Selection of model structure and parameter estimation jointly make up model calibration, discussed in Section 3.7. Before calibration, the methods for finding the structure and parameter values have to be selected.

3.5. Choice of how model structure and parameter values are to be found

In finding the structure, prior science-based theoretical knowledge might be enough to suggest the form of the relations between the variables in the model. This is often implicitly assumed to be so, even in complicated environmental systems where it is not. Shortage of records from a system may prevent empirical modelling from scratch and force reliance on scientific knowledge of the underlying processes. Choice of structure is made easier by such knowledge, and it is reassuring to feel that the model incorporates what is known scientifically about the parts of the system. However, empirical studies frequently find that a much simpler structure is adequate for a specified purpose. In some instances the structure may be found by trial and error among a modest number of possibilities, on the basis of credibility of model behaviour. Structural parameters, such as dynamical order or number and location of spatial subdivisions, may sometimes be treatable as extra parameters to be estimated along with the others. Parsimony (Occam's razor) is an overriding principle: avoid more complication than is necessary to fulfil the objectives.

The next choice is of how to estimate the parameter values and supply non-parametric variables and/or data (e.g. distributed boundary conditions). The parameters may be calibrated all together by optimising the fit of the model outputs to observed outputs, or piecemeal by direct measurement or inference from secondary data, or both. Coarse parameter values indicating presence or absence of a factor or the rough timing of a seasonal event, for instance, might be found by eliciting expert opinion.

The choices of how to put the model together must take account not only of what data can be obtained, but also of its informativeness. Substantial quantitative data may be needed to identify parameter values even in a model with a very simple structure. Jakeman and Hornberger (1993) show how few parameters can be identified sharply from daily streamflow data. Substantial trial and error may be required to discover how much can be adequately modelled from a given data set.

In order to ensure uniqueness of parameter estimates, structural identifiability analysis has been undertaken quite actively in a few environmental system types, including activated sludge biochemical systems (Petersen et al., 2003; Checchi and Marsili-Libelli, 2005). Structural identifiability (Bellman and Åstrom, 1970) concerns what parameters can be identified, in principle, without ambiguity in the absence of measurement errors or deficiencies in model structure.

3.6. Choice of estimation performance criteria and technique

The parameter estimation criteria (hardly ever a single criterion) reflect the desired properties of the estimates. For example we might seek robustness to outliers (bad data), unbiasedness and statistical efficiency, along with acceptable prediction performance on the data set used for calibration. A great deal of effort in recent decades has gone into developing parameter-estimation algorithms with good theoretical properties (Norton, 1986; Söderström and Stoica, 1989; Ljung, 1999). Some of them make quite restrictive assumptions, not always realistic and verifiable, about the properties of the system and the imperfections in the data. Two texts that consider pertinent non-linear theory, at least from a regression analysis perspective, are Bates and Watts (1988) and Seber and Wild (1989).

In selecting an estimation algorithm, rounding errors and ill-conditioning may be a worry, especially when there is a risk that more parameters are being estimated than justified by the data. A further risk is numerical instability, which can arise through injudicious implementation of an algorithm that is stable and well-conditioned in another, exactly algebraically equivalent, implementation. An instance occurs among optimal smoothing algorithms to estimate time-varying parameters (Norton, 1975).

Well executed general-purpose parameter estimation (identification) packages and more specialised packages for hydrological and other uses have now been available for many years (e.g. Ljung, http://www.mathworks.com/products/sysid; http://www.mathworks.com/products/neuralnet). They may not be able to handle complex, integrated models with specialised structures. If, as a result, parameter-estimation software has to be written, careful testing of the model against criteria not used in the estimation is essential for at least three reasons. First, parameter-estimation algorithms are often predictor-correctors, capable of giving plausible results in the presence of coding errors. Second, parameter estimation for complex models usually involves non-convex numerical optimisation, with a risk that the global optimum is not found. Third, a model, especially one that is put together from several submodels, may well have more parameters than necessary to prescribe its overall behaviour (over-parameterisation), and may thus not be capable of yielding well-defined estimates of all parameters. Over-parameterisation can lead to misinterpretation, numerical ill-conditioning, excessive ability to fit the "noise" (inconsistent behaviour) in records and poor prediction performance.

In summary, the parameter estimation technique should be:

- computationally as simple as possible to minimise the chance of coding error;

- robust in the face of outliers and deviations from assumptions (e.g. about noise distribution);
- as close to statistically efficient as feasible (as reflected by the amount of data required for the estimates to converge);
- numerically well-conditioned and reliable in finding the optimum;
- able to quantify uncertainty in the results (not at all easy, as the underlying theory is likely to be dubious when the uncertainty is large); and
- accompanied by a test for over-parameterisation.

In an integrated model, a second area of choice for parameter estimation at this stage is of the sections into which the model is disaggregated. Disciplinary boundaries often define sections, for example hydrological, policy, economic and ecological components. Spatial sectioning, e.g. of a stream network, is also natural. Sectioning into time segments is much less common, even though many environmental phenomena have time-varying characteristics which should influence model applications such as prediction.

The last decade or so has seen a strong trend towards models explicitly divided into simpler sections for parameter estimation, an example being piecewise linear models. Simpler sections make for greater flexibility and easier testing, but pose a larger risk of producing a model more elaborate than necessary, e.g. having internal variables with little influence on external behaviour or higher resolution than needed to provide the required output resolution.

Practical convenience often dictates piecemeal identification of model components, and pre-existing models are often available for parts of the system (e.g. rainfall-runoff, flood, groundwater and/or water quality models for hydrological sections), but it is wise to test the overall model to see whether simplification is possible for the purposes in mind. Sensitivity assessment (Saltelli et al., 2000) plays a large rôle here.

3.7. Identification of model structure and parameters

Section 3.5 discussed choice of methods for finding model structure and parameters, and Section 3.6 the criteria and techniques. The present step addresses the iterative process of finding a suitable model structure and parameter values. This step ideally involves hypothesis testing of alternative model structures. The complexity of interactions proposed for the model may be increased or reduced, according to the results of model testing (steps 3.8–3.10). In many cases this process just consists of seeing whether particular parameters can be dropped or have to be added.

Formal statistical techniques for differentiating among different model structures are well developed. They provide criteria which trade the number of parameters against the improvement in model fit to observations (Veres, 1991). Because of their reliance on statistical assumptions, statistical model-structure tests are best treated as guides, checking the results of the structure recommended on other grounds such as prediction performance on other data sets, credibility of parameter estimates and consistency with prior knowledge (see Sections 3.8 and 3.10).

The underlying aim is to balance sensitivity to system variables against complexity of representation. The question is whether some system descriptors, for instance dimensionality and processes, can be aggregated to make the representation more efficient, worrying only about what dominates the response of the system at the scales of concern. Again it is important to avoid over-flexibility, since unrealistic behaviour, ill-conditioning and poor identifiability (impossibility of finding unique, or well enough defined, parameter estimates) are severe risks from allowing more degrees of freedom than justified by the data.

3.8. Conditional verification including diagnostic checking

Once identified, the model must be ‘conditionally’ verified and tested to ensure it is sufficiently robust, i.e. insensitive to possible but practically insignificant changes in the data and to possible deviations of the data and system from the idealising assumptions made (e.g. of Gaussian distribution of measurement errors, or of linearity of a relation within the model). It is also necessary to verify that the interactions and outcomes of the model are feasible and defensible, given the objectives and the prior knowledge. Of course, this eighth step should involve as wide a range of quantitative and qualitative criteria as circumstances allow.

Quantitative verification is traditionally attempted, but rarely against a wide range of criteria. Criteria may include goodness of fit (comparison of means and variances of observed versus modelled outputs), tests on residuals or errors (for heteroscedasticity, cross-correlation with model variables, autocorrelation, isolated anomalously large values) and, particularly for relatively simple empirical models, the speed and certainty with which the parameter estimates converge as more input-output observations are processed.

Qualitative verification preferably involves knowledgeable data suppliers or model users who are not modellers. Where the model does not act feasibly or credibly, the assumptions, including structure and data assumptions, must be re-evaluated. Indeed, this stage of model development may involve reassessment of the choices made at any previous stage. Checking of a model for feasibility and credibility is given little prominence in the literature because it is largely informal and case-specific, but it is plainly essential for confidence in the model’s outputs. Again this is a very important step, not only to check the model’s believability, but to build the client’s confidence in the model. It assumes sufficient time for this checking and enough flexibility of model structure to allow modifications. Often these assumptions are not met.

3.9. Quantification of uncertainty

Uncertainty must be considered in developing any model, but is particularly important, and usually difficult to deal with, in large, integrated models. Beven (2000) expresses the concept of model equifinality, recognising that there often is a wide range of models capable of yielding similar predictions. Uncertainty in models (Walker et al., 2003) stems from incomplete system understanding (which processes to include, which processes interact); from imprecise, finite and often sparse data and measurements; and from uncertainty in the baseline inputs and conditions for model runs, including predicted inputs. In Van der Sluijs et al. (2005) uncertainties are considered from a non-technical standpoint, to include those associated with problem framing, indeterminacies and value-ladenness. Their procedure is important if these attributes dominate. A diagnostic diagram can be used to synthesize results of quantitative parameter sensitivity analysis and qualitative review of parameter strength (so-called pedigree analysis). It is a reflective approach where process is as important as technical assessments.

Some modelling approaches are able explicitly to articulate uncertainty due to data, measurements or baseline conditions, by providing estimates of uncertainty, usually in probabilistic form such as parameter covariance. Others require comprehensive testing of the model to develop this understanding. Ideally the model would be exercised over the whole credible range of every uncertain input and parameter, suitably weighted by likelihood. Such comprehensive testing is a complex task even for relatively simple integrated models, so is very rarely performed because of time and resource constraints. For example, the sensitivity of model outputs to changes in individual parameters, and perhaps two at a time, may be tested, but analysis of the effects of bigger combinations of parameter changes is usually limited to crude measures such as contribution to mean-square variation in output, under some statistical assumptions. Funds are seldom available to cover the time that this testing takes, but even some crude error estimates based on output sensitivity to the most important variables is useful. Often modellers do not provide even this level of uncertainty estimation.

The results from extensive sensitivity testing can be difficult to interpret, because of the number and complexity of cause-effect relations tested. To minimise the difficulty, clear priorities are needed for which features of which variables to examine, and which uncertainties to cover. A good deal of trial and error may be required to fix these priorities.

Few approaches explicitly consider uncertainty introduced by the system conceptualisation or model structure. Alternative structures and conceptualisations are unlikely to be examined after an early stage. The reasons include preferences of the developer, compatibility with previous practice or other bodies' choices, availability of software tools, agency policy, peer pressure and fashion within technical communities, and shortage of time and resources. It is hard to see how this sort of uncertainty can be taken into account beyond remaining alert to any compromises and doubts in such choices.

On the positive side, the issue of uncertainty is widely recognised and increasing resources are being devoted to it. For example, Hession and Storm (2000) demonstrate a method for incorporating uncertainty analysis in watershed-level modelling and summarise a lot of the literature in this applied area. A recent special issue of this journal (Jolma and Norton, 2005) is also indicative of the attention given to uncertainty in environmental modelling. The papers there illustrate the breadth of the field and the eclectic way in which ideas, problem formulations and technical resources from many sources are being brought to bear.

Model uncertainty must be considered in the context of the purposes of the model. For example, discrepancies between actual output, model output and observed output may be important for forecasting models, where cost, benefit and risk over a substantial period must be gauged, but much less critical for decision-making or management models where the user may be satisfied to know with knowing that the predicted ranking order of impacts of alternative scenarios or management options is likely to be correct, with only a rough indication of their sizes.

3.10. Model evaluation or testing (other models, algorithms, comparisons with alternatives)

Finally the model must be evaluated in the light of its objectives. For simpler, disciplinary models, a traditional scientific attitude can be taken towards "validation" (non-falsification or provisional confirmation, strictly). That is, confirmation is considered to be demonstrated by evaluating model performance against data not used to construct the model (Ljung, 1999, ch. 16; Söderström and Stoica, 1989, ch.11). However, this style or level of confirmation is rarely possible (or perhaps even appropriate) for large, integrated models, especially when they have to extrapolate beyond the situation for which they were calibrated. If so, the criteria have to be fitness for purpose and transparency of the process by which the model is produced, rather than consistency with all available knowledge. More detailed assessment of the model 'for the purposes for which it has been constructed' must be considered (e.g. Ravetz, 1997).

Details of such an approach are still at an early stage of development, but should extend to: testing the sensitivity of the model to plausible changes in input parameters; where possible or desirable, changes in assumptions about model structure; as well as documentation and critical scrutiny of the process by which the model has been developed, including the assumptions invoked. A critical difference from traditional model "validation" is the openly subjective nature of such criteria.

Fitness for purpose should also include 'softer' criteria like ability to accommodate unexpected scenarios and to report predictions under diverse categories (by interest group, by location, by time, etc), and speed of responding to requests for modified predictions. In other words, model accuracy (the traditional modeller's criterion) is only one of the criteria important in real applications.

In summary, the modelling process is about constructing or discovering purposeful, credible models from data and prior knowledge, in consort with end-users, with every stage open to critical review and revision. Sadly, too often in reality it is the application of a predetermined model in a highly constricted way to a problem, and to the social dimensions of which the modeller is oblivious.

4. Minimum standards and education

We conclude by noting that certain minimum standards suggest themselves in reporting on model development and performance and in progressing knowledge. Aber et al. (2003) summarise a workshop discussion on much-needed standards, such as exist for ecological data, of practice for review and publication of models in ecology. They relate to reporting on model structure, parameterisation, testing and sensitivity analysis. Hoping to cover a wide range of modelling situations, we recommend that the standards include (but may not be limited to):

- clear statement of the objectives and clients of the modelling exercise;
- documentation of the nature (identity, provenance, quantity and quality) of the data used to drive, identify and test the model;
- a strong rationale for the choice of model families and features (encompassing alternatives);
- justification of the methods and criteria employed in calibration;
- as thorough analysis and testing of model performance as resources allow and the application demands;
- a resultant statement of model utility, assumptions, accuracy, limitations, and the need and potential for improvement; and quite obviously but importantly;
- fully adequate reporting of all of the above, sufficient to allow informed criticism.

Adoption of these standards by modellers, through fuller execution and reporting of the steps outlined in this paper, would benefit both the model-building community and those relying on model-based insight and model recommendations to make decisions.

In addition to adhering to standards, the education of modellers on further aspects is warranted, for instance on how to engage with clients and stakeholders, on the need to develop more flexible models and on understanding the context in which the model will be used.

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