14. DANISH GROUNDWATER MODELLING GUIDELINES

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14.1 History

Historically, there is no tradition for a rigorous model validation in Denmark. Thus, previous major research projects involving modeling:

- Suså Project (1977-81): National need for methods to predict the consequences of man’s influence on the hydrological cycle (Suså river basin on Sjælland)
- Karup Project (1983): Investigation of the hydrological consequences of irrigation for the Karup river basin (in Jylland)
- The NPO Research Project (1986-91): Modelling of nitrate migration in regional aquifers, nitrate reduction processes and nitrate migration in unconfined alluvial aquifers and in confined limestone aquifers
- Landfill Leachate Polluted Groundwater (1987-92): Field studies at an old landfill, laboratory studies and modelling

A systematic model validation procedure like the ones proposed in the draft Danish guidelines, has not been an issue at all for the listed examples.

The first attempt to introduce best practices in Denmark was taken in the mid 1990’s when a model database for the Copenhagen area was established. The database should allow a better coordination of the various model projects in the area (15-20 setups, some with major overlap). It consisted of both the model setup files and a brief QA document, which described background, objectives, code selection, setup, calibration, simulation and reporting. The idea was that the QA brief (max 10 pages) should describe the overall quality of a given model in a compressed form, and only based on a template / checklist.

The experience with the database showed that the QA brief document introduced a good overview of the quality of a given model even though there were also severe limitations. More information was required (eg. a standard report) in order to evaluate the possibilities of “reuse” of a given model for other modelling purposes. Furthermore, some legal limitations (ownership of certain model setup files) were identified, which limited the possibilities of a free exchange of model setups. Of the 15-20 imported setups in the database only 1-2 were exported and reused.

It was realised, based on the experiences with the model database, that the database and the QA briefs gave a good overview of what was going on. That was a successful result. The exercise also demonstrated, that more focus should be put on QA in order to ensure a common terminology for communication between water resource managers, code developer and model users. Finally, it became obvious that the proposed indicators for characterisation the quality of a given model, could not stand alone. It was not sufficient to characterise the quality at the time of reporting the model and database to
the manager with a brief document. More thorough QA was required during the entire project, from the very start, if transparency and reproducibility were to be increased. Performance indicators (both quantitative and qualitative) had to be introduced and used routinely. More emphasis on describing the conceptual model was required. A procedure for validation had to be developed and a standardised and extended model reporting was necessary.

The construction of the national water resource model (DK-model) in the late 1990’s brought some more systematic procedures. Definition of performance criteria before the calibration was initiated, introduction of inverse modelling in the model calibration process, and the use of quantitative performance indicators in validation tests, were some examples of attempted improvements in the methodology (Henriksen et al., 2002). Even though the DK-model illustrated some possible and useful QA elements, the project also clarified other problems, where new QA initiatives were necessary. One example was incorporation of uncertainty analysis, which could provide information about model structure, parameter, or input uncertainty and significance for model simulations. Another example was the problem of the changing from one model type to another (eg. from stationary to transient model, or from flow to solute transport model).

Numerical groundwater models have been used increasingly in Denmark in recent years both in the planning and management of groundwater protection and in other fields. In 2001 draft guidelines were developed for groundwater flow modelling (Henriksen et al., 2001a). These guidelines were an extract of a comprehensive Danish handbook for groundwater modelling, prepared during 2000-2001 (Henriksen et al., 2001b) as course materials for a basic groundwater modeling course for people from Danish county councils or waterworks, working as regional water resource managers. Groundwater protection, monitoring and resource management were basic elements in this handbook.

The same has been the case for numerous modeling projects for regional authorities, during the past decade:

- Groundwater management (in relation to abstraction licences)
- Groundwater resource assessment (yield estimates)
- Delineation of groundwater capture zones for wellfields (protection issues)
- Solute transport models for evaluation of impacts from point sources / remediation
- Integrated models for groundwater and surface water management and planning (examples from different county councils)

In relation to ongoing groundwater protection activities in Denmark in recent years, a more strict QA procedure has been adopted (see examples in Table 14.1).

### 14.2 Motivation

Before the guidelines were introduced in Denmark there had been a perception among end-users that model capabilities may have been “over-sold”. There was also a lack of consistency in approaches, communication and understanding among and between modellers and end-users, which often resulted in considerable uncertainty for decision-making.
Experiences from model projects in the last couple of years in Denmark showed that county councils (water resource managers) did not find that quality was good enough. Deliverables often did not meet the expectations. Consultants (model users) often found that the expectations in the final model from the county did not correspond to the expectations formulated during the initial phases of the project. Sometimes, the counties had unrealistic expectations to what could be achieved or accomplished by a numerical groundwater model. In some projects, errors or limitations in the selected code had been identified and disputed between model user and code developer. Sometimes, model code developers had the opinion that the model team who developed a site-specific model, did not use the selected code appropriately or correctly.

The guidelines were intended in order to promote constructive dialogue between the client (water resource manager) and the consultant (model user) by clearly identifying up-front the issues most important in the modelling process. It was recommended that a series of meetings should take place during the model study to review progress and milestones.

The guidelines can to a large extent be applied to solute transport modeling in relatively simple, advective-dominated systems. However, the guidelines are not applicable to systems where solute transport is governed by complex chemical and biological processes. For example, the processes governing the transport of reactive solutes are not well understood. Therefore it is difficult to establish modeling guidelines for reactive transport when the fundamental conceptual and mathematical models describing relevant processes need further development.

The draft guidelines are going to be further extended and adjusted in 2003 with additional description of determination of performance criteria, uncertainty analysis,
application of solute transport models etc. before they will be adopted by Danish Environmental Protection Agency.

14.3 Contents of QA guidelines

14.3.1 Principles

The Danish groundwater modeling guidelines are based on a modeling protocol that is widely accepted by the international community (figure 14.1). The guidelines provide a framework within which issues relevant to model development, calibration, testing and predictive simulations should be evaluated and reported. The guidelines can also be used to promote a constructive dialog between model user and water resource manager especially when passing important milestones. It is recommended that a series of meetings take place during the modelling study, to review progress and milestones in the following main steps:

- Conceptual model development
- Model setup and definition of performance criteria
- Calibration and validation
- Simulation and uncertainty analysis

The most important document in the entire model study is probably the tender document. Ideally, the tender document should define requirements for accuracy of the final model. In practice, it is not possible to specify very detailed performance criteria up-front. Wishes for a given accuracy is often dependent on the related costs to achieve a specific level of accuracy. Hence, splitting up the model study into phases, with reviews and adjustment of requirements for subsequent phases, based on what can be agreed upon and achieved, is in practice a more pragmatic and often necessary approach.

QA can not be reduced to a question of numbers. Not everything can be measured or evaluated by quantitative performance indicators. Quality of a given model is also a question of the ability of the model to simulate a given pattern or dynamics, and how the realistic calibrated parameters are. “Pattern reliability” which can be based on a comparison of the simulated and observed groundwater head distribution, is not always reflected by calculated residual head statistics. The same may be the case for dynamic variations in streamflow or groundwater level, where it is difficult to identify perfect indicator or a “suite of perfect indicators” covering both high and low flow conditions. It is often necessary to include more qualitative measures like specialist interpretation of graphical illustrations. Such qualitative criteria can be evaluated by external reviewers.

Another qualitative aspect of models may be an evaluation of the calibrated parameters. Do they have realistic values (compared to predefined ranges)? In model studies where this may not be the case for all parameters, this could be an indication of the quality of the conceptual model, or the lack of the same, due to severe misinterpretations of model structure or geology. Hence, a constructive dialogue between water resource managers and model users is required, and it is often a good idea to have formalised reviews with participation of external experts in order to view and judge the quality of a given model from as many point of views as possible.

Even though it normally is an advantage to split model projects into phases (milestones) it is in practice often not possible to finalize a given milestone, before having moved forward in the process, into the middle of the next phase. In some cases it can be a good idea to run all steps in the model protocol several times, before a satisfactory model has been achieved (Henriksen et al., 2002). In other cases different
phases should be operated in a parallel process, allowing a stepwise building of more complexity into the model.

Figure 14.1 Danish model protocol (Henriksen et al., 2001a)
Where different partners are working together in a model team consortium (one team working with data collection and the conceptual model and another team working with numerical model) or where different domains have to be integrated (root zone model <> groundwater model <> surface water model <> habitat model <> socioeconomic model) a parallel process may also be more convenient in order to exchange information about various steps: conceptual model, model setup and performance criteria, validation test results and simulation uncertainty.

Table 14.2 shows the estimated requirements of a review procedure for different types of models (screening, engineering calculations and aquifer simulations):

| Table 14.2 Review requirements for different model complexity (screening, engineering calculations and aquifer simulation) |
|-----------------|-----------------|-----------------|
| Milestone 1     |                  |                  |
| Conceptual model| Screening        | Engineering      |
|                 |                  | calculations     |
|                 | Model appraisal  | Peer review      |
| Milestone 2     |                  |                  |
| Model setup and performance criteria | Model appraisal | Peer review |
| | None            | Peer review      |
| Milestone 3     |                  |                  |
| Calibration and validation | Peer review | Peer review |
| | Peer review    | Model audit      |
| Milestone 4     |                  |                  |
| Simulation and uncertainty analysis | None           | Peer review |
| |                  | Model audit      |

In the Danish guidelines a standard model report is proposed following a specified chaptering. There has not previously been a tradition for standard model reports - often only a reporting of simulation results has been included. However, it is recommended to put more emphasis on development of standard report in order to communicate the achieved system understanding, validation test results, significance of uncertainties and proposals for future data collection and model refinement.

14.3.1 14.3.2 Brief summary description

The Danish guidelines consist of 49 formulated short guidelines (Henriksen et al, 2001a) extracted from the comprehensive handbook describing best practises (Henriksen et al., 2001b) covering the various steps (figure 14.1):

1. Terms of reference for study
2. Splitting project into milestones
3. A model is a “creative” product
4. Formalised review
5. Standard model report
6. Content of tender document
7. Definition of objectives for model simulations
8. Development of geological model
9. Interpretation of 3D geological models
10. Delineation of model study area
11. Selection of conceptual model complexity
12. Formulation of alternative conceptual models
13. Review of milestone 1 (conceptual model)
14. Selection of model code
15. Starting simple and building more complexity into model
16. Analysis and definition of boundary conditions
17. Selection of horizontal discretization
18. Selection of vertical discretization
19. Parameter estimation procedures
20. Selection of initial values (stationary model/length of hot start period in transient modeling)
21. Pre-processing of rainfall data
22. Pre-processing of potential evapotranspiration
23. Estimation of net-precipitation
24. Pre-processing of groundwater abstraction
25. Pre-processing of groundwater level data
26. Pre-processing of river discharge data
27. Review of milestone 2 (model setup and performance criteria)
28. Using a calibration protocol
29. Evaluation of observation data sets
30. Preparation of observation data sets for calibration
31. Quantification of possible errors and uncertainties related to observation data sets
32. Definition of performance criteria
33. Selection of calibration parameters
34. Manual calibration procedures
35. Automatic calibration procedures
36. Journal of calibration run results
37. Reporting of optimized parameters
38. Validation procedures
39. Free and fixed parameters (risk of “overparameterisation”)
40. Validation of stationary model
41. The analysis of poor validation test results and what to do about it
42. Review of milestone 3 (calibration and validation)
43. Predictive simulations: Selection of a proper reference simulation
44. Groundwater recharge simulation
45. Sensitivity analysis
46. Evaluation of uncertainty related to model structure / geology
47. Content of a model report for aquifer simulation (chapters 1-12 + appendixes)
48. Updating a regional model based on local model studies
49. Review of milestone 4 (simulation and uncertainty analysis)

The guidelines which have been proposed for groundwater flow modelling can to a large extent be applied to solute transport modelling in relatively simple, advective dominated systems.

It is difficult to establish guidelines for all aspects of modelling due to lack of consensus or standard best practices. Further development of model guidelines is considered in the following areas:

- Determination of performance criteria (required accuracy for calibration and validation)
- Uncertainty analysis (data needs, methods for the quantification of uncertainty)
- Reliability of parameters in transient models partly optimised by stationary calibration
- Application of solute transport models
- Scale problems (going from local scale to regional scale and vice versa)
14.3.3 Domains covered

The guidelines are to be applied for new groundwater flow modelling studies and reviews of existing models. Solute transport modelling methodologies are within the scope, but only when dealing with relatively simple, advective dominated systems.

The Danish guidelines are focused on use of models for assessment of water balance, groundwater recharge, particle tracking and flow path. Impacts on flow system from groundwater abstraction is included in the guidelines. The guidelines have most relevance as best practice for regional modeling (grid size from 100 – 1000 m).

Simulation of exploitable (safe yield / sustainable) groundwater resources and how to include water quality and climate variability have only been addressed very briefly and to a limited extent in the present draft guidelines.

Unsaturated zone modeling, surface water modeling and solute transport modeling including geo-chemical processes (nitrate, phosphorous and pesticides) are not included in the present guidelines. Integrated modeling, coupling, and validation of such models have not been included in detail.

14.3.4 Types of users and roles

In Figure 14.2 is shown the existing situation in Denmark with different roles and responsibilities.
Water resource managers

The main responsibility of the water resource manager is to define objectives and performance criteria for the final model. In addition, the manager shall define requirements for code verification and model validation. In many consultancy studies, performance criteria have not been specified, which may imply that the model user specify the criterium, based on results of the calibration. The tender document shall balance the objectives and performance criteria based on available data and economy. This requires a significant insight in modelling from the water resource manager.

Model user

The model user is responsible for selection of model code (or to confirm the adequacy of the model code suggested by the water resource manager), for model setup, calibration and validation. It is important that the model user provides a detailed validation document in such a way that the reliable area of the model and the accuracy of simulations are accurately described.

The documentation has to be thorough to such an extent that simulations if necessary can be reproduced several years later. The model user and the water resource manager shall jointly evaluate, what should be realistic performance criteria for certain objectives, data and economy. Furthermore, the model user must be aware of limitations in the code and be prepared to join a dialogue with the code developer in order to report user experiences with the code, lack of documentation of code, errors, development needs etc.

Code developer

The main responsibility of the code developer is to develop and verify the model code. It is important that the limitations of the code are documented and tests against analytical solutions are included in that documentation. Since code development is a continuous process, and since complex models can not always be tested against analytical solutions, it is important to update the code frequently and test it routinely against more complex test cases. Even though a model code should have an extensive documentation, there can be doubt regarding the functioning of code, also among more experienced users. Active support and dialogue between model user and code developers is thus vital in order to assure the operational model is used on a high professional level.

14.3.5 Types of application

Typical model purposes include:
- Improving hydrogeological understanding and synthesis of data (planning)
- Aquifer simulation and evaluation of aquifer behaviour (planning)
- Evaluating recharge, discharge and aquifer storage processes (assessment)
- Prediction of impacts of alternative hydrological or development scenarios (decision support)
- Quantifying the sustainable yield (assessment)
- Prediction of impacts of alternative ground water protection action plan scenarios (decision support)
- Advection-dispersion solute transport modeling of fate and transport from point sources, including evaluation of various remedial actions (decision support)

14.3.6 Types of jobs

There are three main classifications of model complexity (in order of increasing complexity) in the Danish guidelines:
- Screening model – a simple model suitable for preliminary assessment (rough calculations), not requiring substantial resources to develop, but not suitable for complex conditions or detailed resource assessment. This type of job only requires
limited weight on residuals between model and observations, and does not require a
large amount of data
- *Engineering calculations* – a moderately complex model, requiring more data and a
better understanding of the dynamics of groundwater systems. The type is suitable
for predicting the impacts of proposed developments or management policies.
Increased performance is required for this medium type of job, but a very good
performance may not be necessary. An example of such a type of job is evaluation
of need for supplementary data collection, eg. in an initial phase of a larger project.
- *Aquifer simulation* – a comprehensive model, suitable for predicting responses to
arbitrary changes in hydrological conditions, and for developing sustainable resource
management policies for aquifer systems under stress. This type of job requires the
most strict definition of performance criteria and QA. Examples of jobs is
simulation of groundwater head distribution, flow and concentration in space and in
time, decision support for action plans with focus on land use regulation or other
actions. These types of jobs directly focus on reliability and accuracy, and are often
named “high fidelity” models in english literature.

14.3.7 Supported tools
Software tools have not been developed for the Danish Guidelines. No checklists
have been included in the present draft guidelines. Only for the model database for the
Copenhagen area has the use of brief checklists been introduced, but with limited
success.

14.4 Experience from use of the QA guidelines

14.4.1 Evaluation
- The guidelines have had considerable use in Denmark; end-users has been engaged
  in developing the guidelines (ownership)
- The quality in modeling has been improved (eg. inverse modeling is today used
  frequently, which was not the case 2 years ago)
- Some consultant companies have based their in-house standards on parts of the
guidelines (eg. calibration procedure)
- Formal reviews create room for discussions between model user, reviewer and water
  resource manager this leads to better understanding of what the model can be used
  for and of the limitations of the model
- It’s difficult to quantify performance criteria and prediction uncertainty
- Many models deal with quality assurance of the conceptual model (groundwater
  protection issues); integrated modeling and solute transport modelling need further
  experiences and development in the danish guidelines

14.4.2 Lessons learned
- Quantitative performance criteria are difficult to define for different types of jobs
- It takes time to implement the “new standard for documentation / QA” (eg. model
  users have not adjusted proposals / costs fully for modeling under the new
  guidelines)
- Consequences of additional project costs based on negative review comment, may
  be difficult to agree on or to balance with relation to model performance
- More precise guidelines are required for several issues: stationary/transient
  calibration and validation for different types of jobs, guidelines for integrated
  modeling, solute transport modelling etc.
- In many cases reviews have brought in existing knowledge or models, which was
  not initially used by the model user during conceptual model and model setup (eg.
national dk-model, state of the art knowledge about specific hydraulic parameters etc.) phases
- The skills of both the project leader and the entire model user team is more important under the new guidelines, if time schedules and quality assurance shall run smoothly
- Some water resource managers may believe that more model complexity automatically increases the quality of a model, independently of available data and validation test results

Model resource managers often put more emphasis on data and conceptual model which they normally do understand, than on model setup, calibration, and validation, which they may not understand very well or may find more abstract. On the other hand, model users often put more effort on numerical model, and further refinement of a model instead of asking critical questions about existing data, model structure or need for collection of additional data. Formulation of accuracy requirements (performance criteria) and building more reliable models thus is a “bridging” of two different worlds.

Model courses and discussions and engagement with participation from experience groups (between water resource managers), national EPA, researchers and consultants are important measure in order to make further progress in development and use of model guidelines.

Quality assurance of data must be carried out at all stages of a model project. It is of vital importance to adjust modeling objectives and model complexity, if there is a lack of data of good quality and density. On the other hand, evaluation of data is not independently of a given model structure, and the value of different data may change, when changing model structure and complexity. Both data and stakeholders should be in interaction with the model construction process, when passing important milestones.

14.4.3 Possible recommendations

It is difficult to establish very detailed guidelines for some aspects of modelling (e.g. performance criteria, uncertainty analysis, solute transport modelling etc.), due to a lack of knowledge or consensus about the operational use of such methods. This means that we need “flexible” and “open” tools for HarmoniQuA, which allow incorporation further scientific development for those areas, but also provide access to collected knowledge from other studies, from the knowledge database.

Formal reviews create a room for discussions between model team, external experts and client. This means a better understanding of what a model can do and limitations of the model. We have to incorporate and store such experiences and related decisions during the modelling process, and HarmoniQuA should be able to report such “log-book information”.

Quality assurance must be carried out at all stages of a model project, and both qualitative and quantitative performance indicators are key elements. Feed back loops are required after tender document, conceptual model, model setup, calibration, validation and predictive simulations. Best practise in HarmoniQuA must focus on means for better dialogue between water resource manager, model user and model code developer, incorporating external review procedures.

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14.6 References


