Guidelines for documenting the validity of computational modelling software

IAHR

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The following institutions have jointly developed the guidelines described in this publication:

Centro de Estudios y Experimentación de Obras Publicas (CEDEX)
Antionio Lopez 81, 28026 Madrid, Spain

Danish Hydraulic Institute (DHI)
Agern Allé 5, DK-2970 Hørsholm, Denmark

DELFT HYDRAULICS
P.O. Box 177, 2600 MH Delft, The Netherlands

HR Wallingford Limited (HR Wallingford)
Howbery Park, Wallingford, Oxfordshire OX10 8BA, United Kingdom

Laboratoire Hydraulique de France (LHF)
6 quai Watier, 78400 Chatou Cédex, France

Laboratório Nacional de Engenharia Civil (LNEC)
Avenida do Brasil 101, 1799 Lisboa Codex, Portugal

Norwegian Hydrotechnical Laboratory (NHL)
N-7034 Trondheim, Norway

SOGREAH Ingénierie
P.O. Box 172, 38042 Grenoble Cédex, France

Water Resources Research Centre (VITUKI)
H-1453 Budapest Pf. 27, Hungary

The authors of this report are:

Dick Dee (ed.) (DELFT HYDRAULICS)
Jean Cunge (LHF/SOGREAH)
Gerard Labadie (LNH)
Antonio Ruiz Mateo (CEDEX)
Martin Mathiesen (NHL)
Roland Price (HR Wallingford)
Maria Santos (LNEC)
Ross Warren (DHI)

Foreword

Recent years have witnessed a proliferation of software packages used in hydraulic research and engineering applications. Computational models of complex physical systems are increasingly available to a large and varied group of users. A great deal of knowledge and skill is being transferred in this way, from experts in various scientific disciplines to consultants, policy makers, and other users. While it is exciting to see the products of our professional activities applied to important technological issues in society, this also places increasing demands on the technical quality of the software. At the same time, flexible, easy-to-use information systems firmly encapsulate the models in sophisticated software shells, resulting in the theoretical basis and technical intricacies tending to remain hidden.

All of this stresses the need to examine and support the validity of the models and of the results they produce. In which situations can a particular model be justifiably applied, and how well do computational results represent the actual physics? To what extent has this been tested? What are the estimated accuracies of predictions, and what is the basis for these estimates? Which are the inherent uncertainties in model calculations and how can they be controlled? What has been done to ensure that the model represents the state of the art in conceptual understanding, numerical implementation, and software engineering?

Answers to such questions are relevant to model developers and users alike. Users are often overwhelmed by a large supply of apparently similar software products. They will undoubtedly welcome the means to be able to distinguish among these products on the basis of technical quality of model concepts, algorithms, and limits of application. Developers – particularly those who operate on a commercial basis – need to justify the price they ask for the use of the software, if they are to compete successfully in a crowded market. They need to explain that which is ‘hidden’ and to demonstrate that this hidden part is essential and no less important than a user-friendly interface.

This report represents an important step toward the development of standard procedures for software validation. It contains a detailed set of guidelines for the documentation of the validation process of a computational model. Application of the guidelines to a particular model will produce a validation document: a collection of explicit statements about a model’s technical quality, backed up by computational and experimental evidence to the extent that is available.

These guidelines were produced in a co-operative effort by ten European hydraulic research institutions, all of which are IAHR members. The management of the institutions listed on the inside cover of this report have agreed to use the guidelines as a basis for validating their newly to be developed software. This means that in time to come their validation documents will have a similar appearance and employ a common terminology, and meet various other requirements as implied by the guidelines. These institutes also requested IAHR to make the guidelines available to others working in the same domain, and to solicit comments on the guidelines themselves and on their application in the preparation of the actual validation documentation.

A useful and important property of the guidelines is that they are based on a comprehensive procedural view of model validation, and that they provide a well-defined framework for the presentation of results. While validation has been a prominent issue in computational science for a long time, a generally accepted methodology has been lacking. Undoubtedly this report does not contain the final word on the issue, but it certainly contributes in a constructive way to the development of a systematic approach to model validation.

Dr Torkild Carstens,
President, IAHR

Standard Validation Document

Definition and Guidelines

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The following pages define and explain the Standard Validation Document for computational models.

The table of contents, preface, and part of the glossary are prescribed elements of the Standard. Boxed test, such as this, is explanatory.

Contents

Appendices

Preface

The preface is a prescribed element of the Standard Validation Document. It explains the scope of the document and describes the hydraulic industry's agreements regarding its contents.

The following text is to be included unabridged in every validation document.

The subject of this document is the validation of a computational model. The term *computational model* refers to software whose primary function is to model a certain class of physical systems, and may include pre- and post-processing components and other necessary ancillary programmes. *Validation* applies primarily to the theoretical foundation and to the computational techniques that form the basis for the numerical and graphical results produced by the software. In the context of this document, validation of the model is viewed as the formulation and substantiation of explicit claims about applicability and accuracy of the computational results.

This preface explains the approach that has been adopted in organising and presenting the information contained in this document.

Standard Validation Documents

This document conforms to a standard system for validation documentation. This system, the Standard Validation Document, has been developed by the hydraulic research industry in order to address the need for useful and explicit information about the validity of computational models. Such information is summarised in a validation document, which accompanies the technical reference documentation associated with a computational model.

In conforming to the Standard, this validation document meets the following requirements:

1. It has a prescribed table of contents, based on a framework that allows separate quality issues to be clearly distinguished and described.
2. It includes a comprehensive list of the assumptions and approximations that were made during the design and implementation of the model.
3. It contains claims about the performance of the model, together with statements that point to the available substantiating evidence for these claims.
4. Claims about the model made in this document are substantial and bounded: they can be tested, justified, or supported by means of physical or computational experiments, theoretical analysis, or case studies.
5. Claims are substantiated by evidence contained within this document, or by specific reference to accessible publications.
6. Results of validation studies included or referred to in this document are reproducible. Consequently the contents of this document are consistent with the current version of the software.
7. This document will be updated as the process of validating the model progresses.

Organisation of this document

Chapter 1 contains a short overview of the computational model and introduces the main issues to be addressed by the validation process. The model overview includes information about the purpose of the model, about pre- and post-processing options and other software features, and about reference versions of the software. Validation priorities and approaches are briefly described, and a list of related documents is included.

Chapter 2 summarises the available information about the validity of the computational core of the model. In this chapter, claims are made about the range of applicability of the model and about the accuracy of computational results. A brief statement regarding its substantiation follows each claim. This statement indicates the extent to which the claim has in fact been substantiated and points to the available evidence.

Chapter 3 contains such evidence, in the form of brief descriptions of relevant validation studies. Each description includes information about the purpose and approach of the study, and a summary of main results and implications.

A glossary and complete list of references are contained in appendices.

A word of caution

This document contains information about the quality of a complex modelling tool. Its purpose is to assist the user in assessing the reliability and accuracy of computational results, and to provide guidelines with respect to the applicability and judicious employment of this tool. This document does not, however, provide mathematical proof of the correctness of results for a specific application. The reader is referred to the License Agreement for pertinent legal terms and conditions associated with the use of the software.

The contents of this validation document attest to the fact that computational modelling of complex physical systems requires great care and inherently involves a number of uncertain factors. In order to obtain useful and accurate results for a particular application, the use of high-quality modelling tools is necessary but not sufficient. Ultimately, the quality of the computational results that can be achieved will depend upon the adequacy of available data as well as a suitable choice of model and modelling parameters.

1 Introduction

Introductory information about the computational model and the validation process.

This chapter alludes to the model as a complete software product, and clarifies the relation of that which is being validated to the rest of the software. It includes brief descriptions of pre- and post-processing options, as well as an explanation of the modular structure of the computational core of the model.

In case the computational core consists of a flexible configuration of different modules, there are two possibilities:

1. this validation document applies to a subset of the modules
2. this validation document applies to all modules

Whichever the case, this should be reflected in the title of the document, and clarified din the sections below.

1.1 Model overview

1.1.1 Purpose

The primary purpose of the computational model, e.g. simulation of hydraulic transients in pipeline systems.

In case this validation document applies to a subset of the computational core, the purpose of that subset should be described here in relation to the purpose of the model as a whole.

1.1.2 Pre- and post-processing and other software features

A brief, integral description of the whole model as a stand-alone piece of software. This includes optional add-on modules, as well as components which do not belong to the computational core of the model but which are essential to the computational model as a whole. Examples of the latter are:

- user interface
- grid generator
- plot generator
- data checking module

Interface options with other computational models can be mentioned here as well.

This is the only place in the validation document where the model is treated as a complete software product, and where items not related to the computational core are addressed. Section 2.5: **Software implementation** pertains only to the computation core of the model.

If a detailed description of any of these items is deemed necessary, it should be done in a separate document or report.

1.1.3 Version information

Relevant version information. Recall the requirement listed in the Preface, that the contents of this document should be consistent with the current version of the software.

1.2 Validation priorities and approaches

Brief introduction to the main issues and approaches in validating this particular model. What are the most crucial questions regarding applicability and/or accuracy for this model, and how does this document help to address them.

1.3 Related documents

Brief description of other documentation that this document relies on, such as the technical reference manual associated with the computational model and other relevant validation documents.

For example, if this validation document applies only to the hydrodynamic module of a model system that includes a separate water quality module, and a validation document is available for the latter as well, this should be mentioned here.

A complete list of references (including the documents mentioned in this section) is contained in Appendix B.

2 Model validity

This chapter summarises all available information pertaining to the validation of the computational core of the model. This includes the assumptions and approximations that were introduced during the design and implementation of the model. It further includes claims about the applicability and/or accuracy of (aspects of) the model, together with statements about the substantiation of those claims.

Whenever possible (specifically in Sections 2.2.1, 2.2.2, 2.3.2, 2.4.2, 2.5.2) the format should be:

> Claim: the model (or, for instances, the numerical schema) does this or that with so much accuracy.
>
> Substantiation: brief argumentation, including specific references to existing literature and/or validation studies summarised in Chapter 3.

The nature of a claim and its substantiation varies depending on the subject, as explained below under the headings of the various subsections in which they appear. Claims should be as explicit as possible and provide useful information about model validity. Substantiation should be thorough but brief, which can be achieved by using references.

Note that substantiation may be incomplete, due to the nature of the claim (e.g. the code is free of bugs), or because the evidence is not (yet) available. In such cases it is important to admit this rather that to ‘invent’ a substantiation that appears convincing.

These claims and substantiations together comprise the essential information in this document. The remainder of the document serves either to provide context (Chapter 1), necessary background material (Sections 2.1, 2.3.1, 2.4.1, 2.5.1, Appendices A and B) or substantiating evidence (Chapter 3).

In case the computation core consists of a flexible configuration of different modules, see the remarks made at the beginning of Chapter 1. If a modular structure exists, and if this document applies to all modules, then this should be reflected as much as possible in the organisation of each individual section described below. That is, each section may be divided into subsections pertaining to individual modules.

In order to permit clear and concise statements in this chapter, it is required to have available a complete and consistent description of the theoretical background for the model. Parts of the present chapter will relay heavily on such a description, which will normally be contained in separate documents. These documents must be accessible to the reader, and they should be mentioned in Section 1.3 **Related documents**.

2.1 Physical system

This section describes the physical system or systems being modelled. This may include the medium (e.g. fluid), the geometric configuration (e.g. a network of open, shallow channels), obstacles or other objects (e.g. structures), phenomena (e.g. lateral discharge, wind stress forcing). The description should be as accurate and as complete as possible, since it serves as a reference for the remainder of this chapter.

The section describes what is being modelled, rather than how it is being modelled. One should, therefore, avoid mention of the model or of a particular modelling approach at this stage.

2.2 Model functionality

This section describes the functionality of the model by referring to specific instances/ configurations of the physical system described in Section 2.1. It consists of claims about what the model is actually able to represent, and (to the extent that this is possible) how well it does so.

For the purposes of this section the model can be regarded as a black box, taking input information and producing computational results. It should not be necessary at this stage to refer to the way in which the model was implemented, i.e. how or why it works.

2.2.1 Applications

This section presents an overview of the domain of applicability of the model. This is done by making claims about the types of practical and realistic situations in which the model can be employed, and showing the nature and quality of the information that the model is capable of generating in those situations.

The purpose of providing the reader with an inventory of application types is that it allows him to quickly recognise whether the model is indeed suitable for the application he has in mind.

Each claim in this section refers to a particular type of model application. It should contain a brief description of a realistic physical situation that the model is capable of representing, together with the purpose of applying the model. Whenever possible, information about the accuracy of computational results should be included as well. In view of the complexity of typical applications, however, claims in this section may tend to be rather qualitative.

Substantiation of a claim is typically be reference to one or more case studies, whose result may be summarised in Chapter 3.

2.2.2 Processes

This section further characterises the domain of applicability of the model. Making claims about the individual physical processes or phenomena that the model was designed to represent does this. The idea is to break down the physics into elements that are as simple as possible, yet still meaningful.

The information contained in this section supplements that in the previous section. It is intended to allow the reader to judge whether or not the model is suitable for the purpose, by considering separately the individual processes that play a role in the application he has in mind.

Each claim in this section refers to a particular process or phenomenon that has been incorporated into the model. It should contain a brief description of the process or phenomenon, possibly in terms of a simple physical situation that clearly illustrates it, and provide explicit information about the model representation and its accuracy.

Substantiation of a claim is typically by reference to one or more examples of model experiments or case studies that clearly demonstrate the model's ability to represent the process or phenomenon in question. Results of such experiments may be summarised in Chapter 3.

2.3 Conceptual model

This section describes technical aspects of the conceptual model that are relevant to the validation process. In particular, it addresses the difference between the conceptual model and the actual physics.

The conceptual model (this term appears in the Glossary) is the mathematical/logical/verbal representation of the physical system described in Section 2.1, and forms the theoretical basis for the computational model. In many cases the conceptual model can be expressed as a set of differential equations, but it may also be algebraic, rule-based or otherwise defined.

It is assumed that a complete technical description of the conceptual model is available in a separate document that should be listed in Section 1.3 **Related documents**. It may be helpful to describe her in one or two paragraphs the essentials of the conceptual model, as an introduction to the following two subsections.

We point out that it is not always straightforward to strictly and unequivocally separate the conceptual model from its algorithmic implementation (see Section 2.4). The author should keep in mind that the main purpose of the separation is to expose and clarify different error sources, and that a certain amount of subjective judgement may be involved.

In spite of these remarks one should avoid reference to implementation aspects (algorithms and/or software) in this section.

2.3.1 Assumptions and approximations

A list of assumptions and approximations that have been introduced into the formulation of the conceptual model.

Examples are: hydrostatic balance, turbulence closure assumptions, the assumption that a flow is effectively one-dimensional, and the approximation of the hydrodynamic effects of a structure by means of a discharge curve.

2.3.2 Claims and substantiations

Claims about the validity of the conceptual model and statements about the substantiation of these claims.

This section serves to defend the choices that were made in formulating the conceptual model (i.e. the assumptions and approximations listed in Section 2.3.1) and to explain the implications of those choices for applicability and/or accuracy. The claims and substantiations in this section should collectively imply that the conceptual model is indeed suitable for modelling the physics described in Section 2.1, and that it leads to the functionality claimed and demonstrated in Section 2.2.

A claim about the validity of the conceptual model, as well as its substantiation, will often be rather general and abstract. For example, a claim regarding the hydrostatic assumption in a hydrodynamic model addresses the appropriateness of this assumption in view of the applications of the model. Substantiation of such a claim might consist of a brief argument about the characteristic scale properties of model solutions, together with specific references to the literature. If substantiation of a claim is difficult or impossible, this should be clearly stated.

2.4 Algorithmic implementation

This section describes technical aspects of the algorithmic implementation that are relevant to the validation process. In particular, it addresses the difference between the algorithmic implementation and the conceptual model.

The algorithmic implementation (this term appears in the Glossary) is the conversion of the conceptual model into a finite set of rules suitable for computation. This may involve spatial discretisation schemes, time integration methods, solution procedures for algebraic equations, decision algorithms, etc.

It is assumed that a complete technical description of the algorithmic implementation is available in a separate document that should be listed in Section 1.3 **Related documents**. It may be helpful to describe here in one or two paragraphs the essentials of the algorithmic implementation, as an introduction to the following two subsections.

When discussing the algorithmic implementation, one should avoid reference to the software that implements it.

2.4.1 Assumptions and approximations

A list of assumptions and approximations that have been introduced in order to convert the conceptual model into an algorithmic implementation.

Examples are: approximation of partial derivatives by finite differences, assumptions about smoothness of the solution, approximations introduced by artificial dissipation (numerical filters), approximations of boundary conditions, assumptions about input data.

2.4.2 Claims and substantiations

Claims about the validity of the algorithmic implementation and statements about the substantiation of these claims.

2.5 Software implementation

This section describes technical aspects of the software implementation that are relevant to the validation process. In particular, it addresses the implications of software implementation choices and techniques for the technical quality of the computational model as a whole.

The software implementation (this term appears in the Glossary) is the conversion of the algorithmic implementation into computer code. This includes coding of algorithms, use of standard mathematical software, design and implementation of data structures, etc. The term software implementation, for the purposes of this document, is limited to the computational core of the model. It does not include pre- and post-processing software, user interfaces or other ancillary programmes associated with the computational model.

Software features that are not part of the computational core can be briefly mentioned in Section 1.1.2 **Pre- and post-processing and other features**, if they are considered to be relevant to the technical quality of the computational model as a whole.

It is assumed that complete documentation of the software implementation is available in a separate document that should be listed in Section 1.3 **Related documents**.

2.5.1 Implementation techniques

A list of choices (tools, techniques, standards) that have been made and procedures that have been followed (Software Quality Assurance) in order to convert the algorithmic implementation into software, to the extent that these choices affect the technical quality of the computational model.

Examples are: the use of software engineering tools and procedures, the choice of programming language, standard input/output interfaces, the nature of software testing procedures that have been carried through.

2.5.2 Claims and substantiations

Claims about the implications of software implementation techniques (listed in the previous section) for the technical quality of the computational model and statements about the substantiation of these claims.

For example, an important claim about the software implementation is that it implements the algorithms correctly. This can be partially substantiated by referring aspects of Software Quality Assurance, testing procedures and evidence based on experience with the model.

Other claims in this section might refer to the ability to run the software on various hardware/ software platforms, performance on these platforms, floating point precision, maintenance aspects, expandability of the code, flexibility of interfaces.

3 Validation studies

This chapter summarises validation studies and contributes to the substantiating evidence for the claims made in the previous chapter.

Each section in this chapter corresponds to a validation study whose purpose can be clearly identified in the context of the material presented in the previous chapter. Such a study may involve case studies, theoretical analysis, comparison with measurements, comparisons with other models, etc, as long as it is relevant to the purpose of the study.

Summaries of studies should contain:

- title of study
- date of study
- date of (last update of) summary
- model name and version information
- description of purpose
- description of approach
- main results
- conclusions and implications for the user
- list of references to reports/publications

A suggested format is described in some detail in a sample subsection on the next page (Section 3.1).

3.1 <sample study>

The following is a suggested format for summarising a validation study. Complete references to verifiable and accessible sources should be listed in Appendix B **References**.

Title
Indicated in section header above. This title will also appear in the Table of Contents of this document. Examples: *Spiralling flow through a curved channel, The effect of curvilinear grid co-ordinates on model accuracy, Numerical smoothing and stability*.

Date of study
The date that the study was performed.

Date of summary
The date that this summary was last updated.

Version
Version information, e.g. the version number of the model that was used in the validation study, possibly other version numbers to which this study applies.

Purpose
One- or two-paragraph description of the main purposes(s) of this contribution to the validation document, clearly placed in the framework provided by this document. Preferably the purpose should be the verification of one of the claims or statements made in Chapter 2 of this document. Note that this may be quite different from the original purpose of the study.

Approach
Summary of validation methods and techniques, experiments performed, etc, in order to achieve the stated objectives. Not too many details; better to point to reports or publications. However, it must be possible to understand the essence of what was done by reading only this text. This means, for instance, that the most important model parameters that were used in an experiment should be listed here.

Results
Summary of results presented graphically whenever this makes sense.

Conclusions
Conclusions that may be drawn from the results. The most important aspects are the implications to the user: how can he use the results of this study to judge model quality in his own application.

A Glossary

This glossary may be expanded by the author(s) of the validation document. However, it should at least contain the following four items.

computational model: software whose primary function is to model a certain class of physical systems. The computational model may include pre- and post-processing features, a user interface, and other ancillary programmes necessary in order to use the model in applications. However, this validation document primarily concerns the core of the computational model, consisting of the underlying conceptual model, its algorithmic implementation and software implementation.

conceptual model: a mathematical/logical/verbal representation of a physical system or process. This representation may involve differential equations, discrete algebraic equations, decision graphs, or other types of conceptual descriptions.

algorithmic implementation: the conversion of the conceptual model into a finite set of rules, suitable for computation. This may involve spatial discretisation schemes, time integration methods, solution procedures for algebraic equations, decision algorithms, etc.

software implementation: the conversion of the algorithmic implementation into computer code. This includes coding of algorithms, use of standard mathematical software, design and implementation of data structures, etc. The term software implementation, for the purposes of this document, is limited to the computational core of the model. It does not include pre- and post-processing software, user interfaces, or other ancillary programmes associated with the computational model.

B References

A complete list of reports, books, manuals, articles, etc, referred to in the text.