Deltares

Enabling Delta Life

Development plan
Water Quality Modelling Framework

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Title
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Summary
Innovation of Deltares' modelling framework for surface water and groundwater quality requires careful planning and co-ordination. On the basis of a roadmap this plan describes the strategy, the issues, the priorities and proposed activities (projects).

References
Deltares strategic R&D programme 2009

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Contents

1 Introduction

1.1 Background

Water quality models have been and are being extensively used by Deltares in many investigations with regard to the behaviour of polluted saline and fresh surface water systems and groundwater systems. Key problems to be studied are the occurrence of eutrophication, nuisance algal blooms, anaerobic conditions, the accumulation and fate of toxic pollutants, bacterial pollution and salination. In recent years attention has been drawn in particular to the role of the interfaces in and between these systems, such as estuaries and bottom sediment, and to the processes in deep stratified water.

Models are being used widely to study the effects of water management and remedial measures, and to help determine cost-effective remediation. Examples of measures are the reduction of nutrient and pollutant loads, the artificial mixing in deep reservoirs and lakes, and the removal or capping of bottom sediment.

Recent developments concern the integrated of groundwater and surface water quality and for “operational water quality management”. There is a great variety of spatial and temporal scales that need to be covered by the models, from very small to large spatial scales, and from very short to long time scales. Required process detail may be quite different for the various scales.

In view of new management questions, changing demands for application, changing insights, ever increasing knowledge, and rapid IT development, the development of the water quality framework (WQMF) needs to be an ongoing process. Moreover, with the merging of four organizations to form Deltares, a great number of water quality packages (also containing ecological components) are now available within the organization, both for surface water and groundwater, that need to be unified and coupled.

Currently, both strategic and applied R&D-projects of Deltares tend to rely on the existing framework, which inhibits its development. The principal reason for this is that strategic research needs as formulated in “SO-vraagsturing” documents mostly relate to the ecological and water quality effects of the use of water resources and of climate change and the effectiveness of measures, and not so much to the tools needed for answering the research questions concerning knowledge development and system understanding. The guiding document for water related strategic research “Nationale kennis- en innovatieagenda Water 2010-2012” (SO-vraagsturing; draft 2 July 2009) contains 23 “needs” for which water quality is an important tool (A4,G9,G17,I2,I8,I9,I18,I19,I20,I25,I26,I27,I28,I29,J7,L3,M4,M6,M7,N6, Q1,P3,P4) and only 3 “needs” that directly concern the development of water quality models (A9,I11,S8). Another important reason for slow development of the WQMF is found in limited financial resources for individual projects.

Nevertheless, the need for innovation and upgrading of the water quality framework arises in many of Deltares’ projects, R&D projects and consultancy projects alike. It is necessary to maintain consistency among the activities in these projects, to tune and combine development activities, and to provide these projects with an efficient, state-of-the-art uniform and integrated framework. Consequently, the development of the water quality framework needs to be planned carefully.

1.2 Objectives

Deltares water quality framework (WQMF) is one of the essential tools being used in its research projects and consultancy projects, and therefore strongly contributes to its position as a state-of-the-art research and consultancy institute. However, in recent years the innovation and integration of components of the WQMF has been lagging behind. Seen from this perspective, the plan for the development of the WQMF needs to provide:

- a basic design of an efficient, state-of-the-art, comprehensive, integrated framework for water quality and basic ecological components;
- a short list of high priority projects for the development of the framework;
- an estimate of the costs of these projects; and
- recommendations for the planning and tuning of water quality development in the present strategic R&D projects of Deltares (SO projects).

The pursued state-of-the-art water quality framework is uniform with regard to process formulations, flexible with regard to process details and provides smooth coupling of models for saline and fresh surface water systems and groundwater systems. Because of these properties the framework will be applicable for all relevant spatial and temporal scales (including models for OMS). The framework will be an adequate basis for systems analysis and knowledge development to address all WFD, MSFD and GWD issues concerning water quality and ecology.

1.3 Study approach

As a first step in the designing of a plan for the WQMF, the contours and the building blocks of the framework have been defined and schematized in a so-called roadmap. This roadmap depicts the coherence of the building blocks and the planned development over time. The map is to be used as a planning tool.

The second step involved an inventory of the development issues based on:

- the needs of water quality related R&D projects (SO and TO) and consultancy projects (SLA and other assignments) of Deltares;
- the knowledge and research questions included in the inventory “vraagsturing 2009”;
- relevant external developments.

Project plans have been studied and project leaders have been interviewed for the inventory.

In a third step the issues have been formulated as sub-projects, that were also prioritized and budgeted.

Finally, an approach of how to integrate the execution of the WQMF sub-projects into Deltares’ strategic research programme (SO) has been formulated.

1.4 Guide to this report

Chapter 2 presents the roadmap and explains the various building blocks and how development is to take place over time.

Chapter 3 contains the actual development plan, starting with the development strategy and an overview of the issues that resulted from the inventory. The plan includes outline proposals for development sub-projects, makes suggestions how distribute them among new SO-programme “Development of WQMF” and existing SO-programmes. The final section provides a tentative cost estimate.

Appendix A lists and describes the development issues for each of the four Deltares units involved in the development of the WQMF as resulting from the inventory. Current planning, financing and priorities are discussed. The background for this is provided in Appendices B-E. The inventory resulted in a number of observations regarding the situation of Deltares’ WQMF and the possibilities for the tuning of relevant ongoing activities. These observations are included under section A-5 of Appendix A.

2 The roadmap

To arrive at an efficient, state-of-the-art, comprehensive, integrated framework for water quality and basic ecological components, the currently available building blocks need to be integrated and innovated, and new components have to be added. A roadmap has been developed as a planning tool for the development of the WQMF (Figure 2.1). This roadmap focuses at the coupling of water quality models for groundwater (MT3D) and surface water (Delwaq) on the basis of a generic processes library and the development of new methodology to enhance and extend application.

The roadmap should be read as follows. The boxes contain building blocks for: components (pink and blue), interfaces with other domains (purple), frameworks (orange) or model applications (green). The arrows indicate how building blocks support other building blocks. At the same time, the arrows indicate the overall direction of the development of the framework. In order to warrant transparancy and readability it was necessary to group boxes in a logical way and to keep them as small as possible. Consequently, the magnitude and position of a box does not show the exact order and duration of development activities for each of the building blocks. Begin and end can be substantially earlier or later than appears from the roadmap. For each of the components, the urgency (priority), the start and the expected duration appear from the development plan and from connected project proposals.

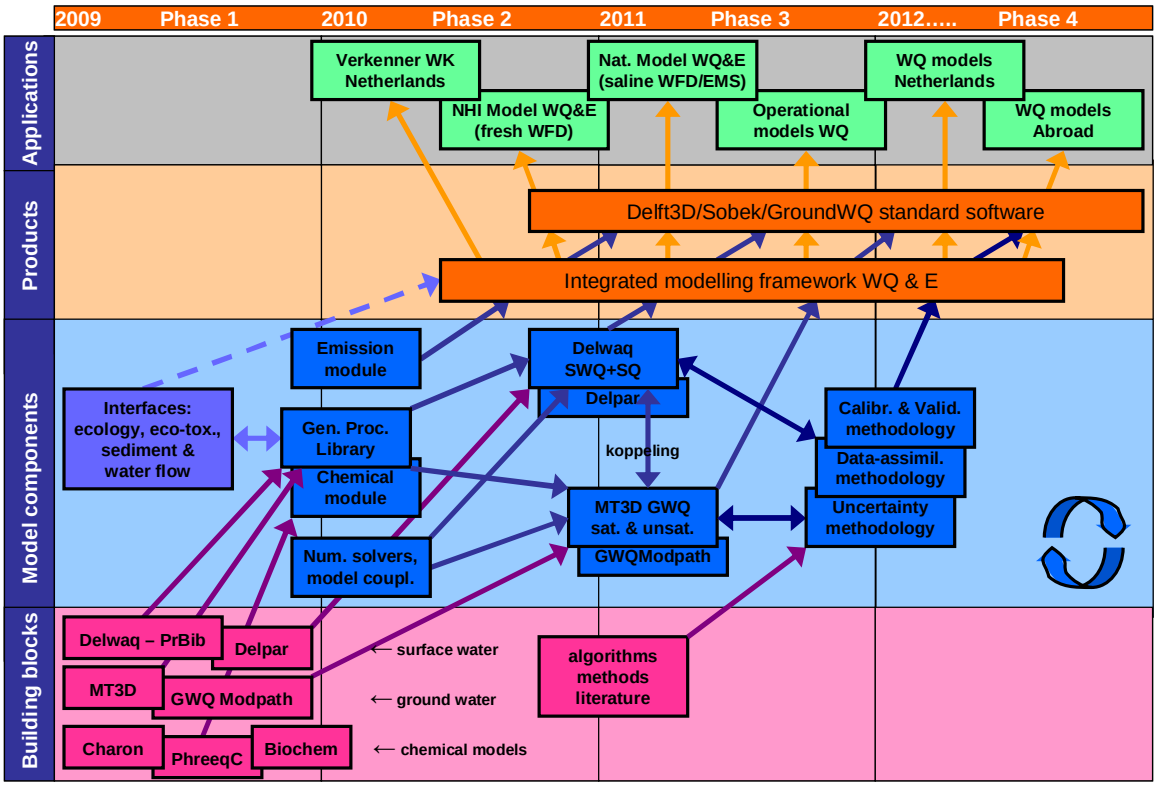

Figure 2.1 Roadmap for the water quality modelling framework (WQMF). Legenda: WQ&E = water quality and ecology; SWQ = surface water quality; SQ = sediment quality; GWQ = groundwater quality; NHI = Nationaal Hydrologisch Instrumentarium; Interfaces = interfaces between WQMF and other modelling frameworks.

Nevertheless, the overall trends in the roadmap are “the lower on the vertical scale, the more remote from the final development stage“ and “the more to the right on the horizontal scale, the longer development may continue”. Generally, developments will be stepwise and cyclic, depending on new demands that turn up. The roadmap shows how a generic, coherent, integrated water quality modelling framework (orange) can be developed starting from the basic components currently available with Deltares (pink). The framework exist in two forms: the collection of building blocks in use and under development by the various units of Deltares (BGS, ZWS, ZKS, etc.), and the standard software packages developed for the commercial market by DSC. Ideally, there will be a continuous inflow of improved and innovated components into the standard software.

Some components, such as Delwaq and the processes library for surface water quality are in an advanced state of development. From a software technical point of view MT3D for groundwater quality is substantially less developed. A host of versions exist that are different in substances, process detail, formulations and software infrastructure. The surface water and groundwater components need to be coupled, both to be fed from the same generic processes library. The interface between the surface water and groundwater models will be at the lower boundary of the macro-biologically active sediment layer. The components for chemical CHARON and PhreeqC may need to be integrated in the generic processes library. CHARON has been implemented provisionally. Biochem coupled to Orchestra, a ecotoxicological management support system, may remain a stand-alone component.

The processes library provides for the coupling of water quality processes with ecosystem components (modules for organisms) that are also part of the library. Currently, this includes modules for phytoplankton, microphytoplankton, grazers, macrophytes and drowned vegetation, that are in various stages of development, ranging from highly developed (algae) to marginally implemented (macrophytes). Modules for bacterial biomass and foodwebs (fish, etc.) are lacking. Such modules form the interface with ecological . Other interfaces that need to be served by water quality processes concern modules that simulate bioaccumulation and ecotoxicological effects.

Hydraulic and hydrodynamic and sediment transport and morphological are also important inputs for water quality . The interaction can be two-directional. There is a tendency to incorporate sediment entirely in Delwaq. Couplings need to be mass conservative.

The flow path models Delpar and Modpath are stand-alone components but partially use the same infra-structure as Delwaq and MT3D.

The emission module for point sources and diffuse sources can be a stand-alone component, that facilitates output on a range of spatial and temporal scales, includes the required aggregation and de-aggregation algorithms, and fits the input formats of Delwaq and possibly also of MT3D.

The building block “numerical solvers and coupling with water flow models” represents the cluster of activities that concern the improvement of the numerical performance and communication of models. The focus will be on the reduction of computational burden, the conversion and aggregation of simulated flow fields.

Three “new” supporting components have been included in the roadmap, namely:

- data-assimilation methodology;
- uncertainty analysis methodology; and
- calibration/validation methodology.

These components are invaluable for water quality for operational management systems and for risk assessment. The latter two components are also very important long term and scenario analysis. Each of the three methodologies is still in its infancy with respect to water quality .

The model applications (green) will be constructed on assignment on the basis of standard software or innovated basic components that have not yet migrated into standard software (orange). Often not only water quality components but also ecosystem components (modules for organisms) will be part of the applications. For strategic reasons, components developed by other parties can be made part of these applications (STONE and ANIMO developed by Alterra, DUFLOW, etc.). Distinction is made between several major applications for the Dutch market, applications for the foreign markets, and models for operational management system (OMS), because systematic differences in components used are encountered. Models for OMSs are used for short term predictions (days), whereas the other application concern long term prediction (years).

3 The development plan

3.1 Strategy

To arrive at an efficient, state-of-the-art, comprehensive, integrated framework for water quality and basic ecological components, the currently available building blocks need to be integrated and innovated, and new components have to be added. A roadmap has been developed as a planning tool for the development of the WQMF (Figure 2.1).

A long time the development of Deltares' water quality framework (WQMF) has relied on small stepwise innovations established in a multitude of research and consultancy projects. This has led to diversion. Activities aiming to tune, to integrate and to consolidate innovations have been lacking. Consequently, in the current development plan for the WQMF the highest priority is given to such activities. Over the coming years priorities will shift to further innovation of the WQMF. Nevertheless, some of these innovations are very urgent, as they have been delayed due to a lack of resources and planning. Such innovations need to start as soon as possible.

Water quality modelling is anything but a stand-alone activity. It has interfaces with the frameworks for hydrological, hydraulic, hydrodynamic, sediment and ecological . The development of couplings of the WQMF with other frameworks will be planned and tuned with the modellers from these other disciplines. More in particular, adequate interfaces with ecological modules in the WQMF need to be established. The water quality modellers will primarily work on couplings and interfaces as they deem fit for the needs of water quality. However, the content of ecological modules and the pace of the integration in the WQMF will be determined primarily by the ecological modellers.

The achievement of state-of-the-art results requires development activities be carried out by specialists. This holds for water quality, but even more for those components in water quality that connect to other disciplines than chemistry, biochemistry, microbiology and mass transport. Ecological modules need to be developed by ecologists, sediment modules by physicists, numerical solvers by mathematicians, parallelization by computer informatics specialists, etc. This makes the development of the WQMF a multidisciplinary task, in which many specialist members of at least four of Deltares' units (BGS, ZWS, ZKS and DSC) will be involved.

Because financial resources are limited, projects have to be carried out purposefully and efficiently. Doing things twice, doing similar things with different tools or working on more than one tool for the same purpose are to be prevented. Priorities must be set in view of the needs according to SO-"vraagsturing", TO and SLA projects and the international market for water quality. Choices between alternative tools must be made. Consequently, the execution of the development plan as implemented in SO-projects and other projects will be managed carefully. This involves yearly updating of the plan and monitoring of progress, tuning and quality of projects.

It should be pursued to include or even integrate as many projects as possible in the existing SO-programmes. This will promote the development of components, tools and methodologies that can be optimally used to address the primary research questions of these programmes.

For the time being the preliminary project proposals in sections 3.3 and 3.4 are described as “stand-alone” projects. Suggestions for the integration in the various SO-programmes (roadmaps) are made in section 3.5. The projects that can not be integrated in these programmes will together shape up the new SO-programme “Development of WQMF”. Opportunities for future integration in knowledge oriented SO will be seized to make this SO-programme as lean as possible. Section 3.6 provides a tentative cost estimate.

3.2 The development issues

In order to warrant coherent execution, the proposed projects (issues) have been grouped according six themes that reflect aims. A priority varying from 1 to 3 has been allocated by the project-team to each of the development issues in view of the needs of Deltares’ ongoing R&D and consultancy projects. The numbers in the list of issues indicate the priority (1, 2 or 3) or the number of an aim (1-6). Priorities 2 and 3 do not mean that working on an issue should wait. The priorities indicate preferences in view of limited financial resources for R&D. However, priority 1 projects should be started ultimately in 2010, as they mostly concern activities that were put on waiting lists in the past years.

1 Coupling of components:

1 Generic and flexible coupling of Delwaq (WAQ/ECO) to MT3D
1 Generic coupling of ANIMO to MT3D

2 Development of new components:

1 Development of a generic emission module
3 Design study for a versatile unsaturated zone module (after go decision)

3 Innovation and standardisation:

1 Development of a generic processes library for surface water and groundwater quality
1 Innovation of the processes library
1 Eutrophication model calibration resulting in default coefficients
1 Publication of calibrations of the models
2 Implementation of the generic processes library in standardised MT3D
3 Development of default coefficients for micro-pollutants

4 Enhancement of computational performance:

1 Parallelization of MT3D and Delwaq
1 Improved coupling with hydrodynamics and hydrology
2 Development of more efficient numerical solvers

5 *Development of supporting methodologies:*

1 Data-assimilation for operational management WQ models;
1 Scaling over space and time for WQ models
2 Uncertainty analysis
3 Calibration and validation methodology.

6 Enhancement of application efficiency:

1 Incorporation of innovations into standard Delwaq
2 Development of UIs for the WQMF
3 Development of tools for mass balance analysis

3.3 High priority projects

The proposed projects are grouped according to the 6 themes. Each thematic project includes several sub-projects. Only outlines of the proposed projects are provided here. Upon the approval of projects and the allocation to the various SO-programmes, detailed project plans will be made.

SO-Project 0: Management of development WQMF

The development plan for the WQMF will be updated yearly by a small project team in which the units BGS, ZWS, ZKS and DSC are represented. The team monitors the progress and quality of all WQMF related sub-projects, and stimulates integration and tuning of the activities for water quality modelling in the various SO-projects and other projects. The team will report quarterly to MT-Knowledge, and will advise with regard to the execution of all WQMF related sub-projects and new sub-project proposals.

SO-Project 1: Coupling of WQ components

1.1 Coupling of MT3D and Delwaq
1.2 Coupling of MT3D and ANIMO

Ad 1.1) The interface of MT3D and Delwaq will be at the interface of the macro-biologically active sediment layer and the deeper sediment/soil. Eventually, coupling will be flexible which implies two-way communication between the models and the possibility of stand-alone application. However, a one-way coupling of MT3D and Delwaq allowing for the transfer of water and substances from groundwater to surface water will be established as a first step. An important issue is parameterization of the effects of sediment/soil heterogeneity and tubing. Benefit needs to be taken from work that has been or will be done in projects such as “Grondwaterbijdrage kwaliteit oppervlaktewater zuidoost Brabant” and “Scaling up of sediment data to grid cell (TNO GIP)”.

Ad 1.2) The existing coupling of ANIMO to RT3D will be reproduced in the “standard” version of MT3D.

SO-Project 2: Development of new WQ components

2.1 Generic emission module

Ad 2.1) The development of the emission module has resulted in a first version. The module will be enhanced and extended to accommodate a wide array of emission conditions and 1-2-3D model settings. This includes the demands of integrated river basin and sea for micropollutants and nutrients, especially with regard to the quantification of emissions from land-based diffuse sources. The GIS-based MONERIS methodology for nutrients will be taken into account.
Re-programming will result in compliance with the new formats of DeltaShell.

SO-Project 3: Innovation and standardisation WQMF

3.1 Development of a generic processes library
3.2 Innovation of the processes library
3.3 Eutrophication model calibration resulting in default coefficients
3.4 Publication of calibrations of the models

Ad 3.1) The generic library will be developed on the basis of the present processes library of Delwaq and its documentation. A design will be made, that allows for both complex and strongly simplified (parameterized) process formulations. Selection can be done through option parameters. An inventory will be made of the MT3D processes to be included. Priority processes can be selected from recent or ongoing projects like “Grondwaterbijdrage kwaliteit oppervlaktewater zuidoost Brabant”, SO-project “Waterbodem beheersstrategieën”, SO-project “Sanerings-technologie organische verbindingen” and PhD project “Verschoor - Metal binding DOC”. The activities include the implementation of formulations in software, and the documentation of the processes.

Ad 3.2) The innovation of the processes library will be driven by the needs that arise in Deltares’ projects. Quite a number of existing modules still need to be integrated into the processes library, but there is also a need for specific extensions. The innovation will be carried out stepwise, as demanded by Deltares’ projects. An inventory resulted in the following topics:

- integration of the floating nuisance algae module (BLOOM), possibly based on more detailed nutrient, detritus and extinction around the thermocline;
- limitation of phytoplankton (BLOOM) by carbon dioxide and uptake of sulphur;
- effects of micropollutants on primary production;
- integration of a helophyte module (nutrients, organic matter);
- integration of dynamic grazer modules (zooplankton and benthic grazers, such as Dreissena);
- integration of CHARON and/or PhreeqC for the simulation of macro-chemistry and pH;
- integration of a macrophyte module (nutrients, organic matter, suspended sediments and light extinction;
- integration of (suspended) sediment formulations;
- effects of macro-chemistry, microphytobenthos and zoobenthos on the cohesiveness and erodability of sediment;

- process formulations ranging from ultimately simplified to complex (also allowing reduced computational burden);
- extension of the number of sediment fractions (dynamically);
- effects of artificial aeration on dissolved oxygen, carbon dioxide and methane;
- fraction simulation with respect to primary emission sources;
- tracer options with regard to floating and settling (available in Delpar not in Delwaq);
- improvement of UITZICHT with regard to secchi depth;
- transition fresh-saline;
- improvement of temperature ;
- growth and mortality of bacterial biomass (especially for MT3D);
- (p.m. integration of a foodweb module such as ECOPATH);
- (p.m. integration of a mesozooplankton-jelly fish module).

CHARON has already been coupled to Delwaq in a provisional way and PhreeqC has been coupled to MT3DMS. A choice may have to be made for reasons of maintenance efficiency and preferred functionality.

Ad 3.3-3.4) The calibration of ECO-Delwaq-G for the Wadden Sea will be completed. Scientific publications will be written, that describe the representative calibrations of the main configurations of the processes library. Examples of calibrations are the still to be published concern the eutrophication model ECO-Delwaq-G for Lake Veluwe and for the Wadden Sea. Other cases may concern Lake Vlietzicht (deep lake, temperate climate) and Upper Peirce Reservoir (deep tropical lake, “SDWA-Deep Lakes”). The resulting sets of process coefficients will be made available as “default” coefficients.

SO-Project 4: Enhancement of computational performance WQMF

The project is composed of the following sub-projects:

4.1 Parallelization of MT3D and Delwaq
4.2 Improved coupling with hydrodynamics and hydrology

Ad 4.1) The main objective of the parallelization of components is to reduce simulation run times. The parallelization of the components for surface water quality, groundwater quality, hydraulics, hydrodynamics and groundwater flow needs to be based on similar methodology and similar software tools. Work has been done for FLOW and Delwaq (3 of the 21 solvers).
The activities will be gathered under one project encompassing the following activities: a) generic design of parallelization, b) development of generic software tools, c) implementation in MT3D solvers, d) implementation in Delwaq solvers, e) implementation in other components (to be specified), and f) testing. The project will be co-ordinated by DSC. Specialist input from DSC is required.

Ad 4.2) The shortcomings that are discovered in existing couplings of Delwaq and hydrodynamic models based on Delft3D-FLOW will be taken away, and new couplings will be implemented. Planned activities concern:

a) the improvement of the stability of FLOW-z-layer and its recently implemented implicit solver; and
b) on-line coupling of FLOW and Delwaq to simulate the interaction of water flow and submerged vegetation due to flow resistance.

The latter requires re-structuring of the core code of Delwaq, which would reduce the need for a separate transport solver in Delft3D and Sobek flow kernels.
A future activity may concern the coupling of Delwaq to a Delft3D-WAVE/SWAN version for shallow lakes.

SO-Project 5: Supporting methodologies WQMF

5.1 Data-assimilation for OMS WQ models
5.2 Scaling over space and time for WQ models

Ad 5.1) Data-assimilation methodology will be developed for salinity, temperature, suspended sediments, algae biomass (chlorophyll), cyanobacterial biomass, dissolved oxygen, nutrients and detritus.in Delwaq. The focus will be on the development of basic methodology and software tools for:

a) the conversion of measured parameters into simulated parameters;
b) the interpolation, extrapolation and scaling of data for concentration fields for computational grids;
c) incorporation of concentration fields into Delwaq models;
d) data-assessment for operational management (decision rules).

Priorities will be derived from Deltares OMS projects. FEWS will be the platform for water quality for operational management. Plug-ins for Delwaq are already available.

Ad 5.2) The scaling methodology is to accommodate both detailed local/regional applications and river basin/national applications of the surface water quality and groundwater quality components (Delwaq and MT3D). A design study is the first step to be made. This study makes an inventory of needs and possibilities, and delivers an approach of scaling and aggregation that covers all relevant spatial and temporal scales. Relations with hydrological and hydrodynamic will be investigated.
Implementation of the methodology is the next step. Because the methodology will probably affect process formulations, process coefficients and input data conversion, it is expected that the deliverables include processes library components, parametrization procedures, data conversion tools and data aggregation tools. With these tools available system data and computed water flows can be pre-processed to fit spatial and temporal scales. In case of stand-alone applications of MT3D and Delwaq a scaling tool to convert MT3D results into Delwaq input may be needed.

SO-Project 6: Enhancement of application efficiency WQMF

6.1 Incorporation of innovations into standard Delwaq

Ad 6.1) The incorporation of innovations of the processes library in the standard Delwaq (Delft3D, Sobek) involves PLCT modification, additional testing and documentation. Priority is given to existing innovations that have not yet been incorporated, such as Delwaq-G. The selection of substances and processes from different groups may need to be made more flexible.

3.4 Projects with lower priority

The projects with lower priority are grouped according to the same six aims. Lower priority does not mean that these projects can wait. It indicates that the projects have lower preferences in view of limited financial resources for R&D.

SO-Project 1: Coupling of WQ components

None

SO-Project 2: Development of new WQ components

2.2 Design of a versatile unsaturated zone WQ model

Ad 2.2) The start of this project dependents on a go/no-go decision in line with a decision on whether Deltares should develop its own unsaturated zone module or should stick with Alterra's ANIMO. Currently ANIMO is the starting point, but it is conceivable that a new start is to be preferred.
A versatile unsaturated zone WQ model would have to include nutrients, organic matter, pesticides, heavy metals and salt. Such a component may provide the emissions from diffuse sources on land into surface water, via both groundwater and run-off. Consequently, the link with Deltares' emission module should be investigated, and the GIS-based MONERIS methodology for nutrients needs to be considered. The design study has to be tuned with the needs of Deltares projects such as "Salt near root zone" (proposal) and SLA "NHI-waterkwaliteit".

SO-Project 3: Innovation and standardisation WQMF

The following sub-projects are distinguished:

3.5 Implementation of the processes library in standardised MT3D
3.6 Development of default coefficients for micro-pollutants

Ad 3.5) The design of processes library also needs to address the implementation of processes back into MT3D. The code of MT3D will be modified to accommodate this and to incorporate other features in a modular way. The many versions of MT3DMS (multi substance), MT3D and RT3D need to be converted into one generic, standardised version, that will be the starting point for the migration of MT3D towards commercially available "Deltares software". MT3DMS being rather modular and rather versatile as to processes is the preferred version, the modification of which may not take a large effort, because it is rather modular and because it contains most of the required features.

Ad 3.6) A database concerning default process coefficients for organic micropollutants (priority substances WFD) will be developed as a tool immediately accessible within Delwaq.

SO-Project 4: Enhancement of computational performance WQMF

4.3 Development of more efficient numerical solvers

Ad 4.3) More efficient numerical solvers will be developed and implemented, that allow for the reduction of the computational burden and run times of spatially detailed and comprehensive Delwaq and MT3D models. Solvers for Delwaq are usually developed in co-operation with mathematics departments of universities. As a first step the new numerical scheme 21 in Delwaq will be adjusted for 3D application.
MT3D and MODFLOW are open-source packages developed and maintained by UGS. The current approach with regard to MT3D is that Deltares does not take initiatives, but will try to benefit from autonomous external developments. Nevertheless, it is conceivable that MT3D can benefit from solvers developed by Deltares for Delwaq.

SO-Project 5: Supporting methodologies WQMF

5.3 Uncertainty analysis
5.4 Calibration and validation methodology

Ad 5.3) The development of methodology for uncertainty analysis of water quality simulation results is in its infancy. The activities will start with literature study and an inventory of promising methods. Selected methods will be implemented in software where possible, directly in Delwaq and/or in pre- and post-processing tools. Pre-processing may involve the determination of probability distributions of input parameters, such as spatially varying decomposition rates (micro-pollutants in groundwater). The implications for risk analysis will be identified.

Ad 5.4) The “goodness of fit” calibration/validation methodology already developed in relation to phytoplankton (BLOOM) will be improved and extended. Relevant calibration tools (filters, etc.) developed in the “DA-Tools-OpenDA-COSTA” project are starting points. A literature study will precede the actual development activities.

SO-Project 6: Enhancement of application efficiency WQMF

6.2 Development of UIs for the WQMF
6.3 Development of tools for mass balance analysis

Ad 6.2) New user interfaces will be developed by DSC for Delwaq, MT3D and the coupled Delwaq-MT3D framework on the basis of generic DeltaShell tools. A start has already been made with a new UI for Delwaq. This is to be extended from 1D applications to 2-3D applications. The input from Delwaq users and MT3D users is required to construct UIs that allow for intuitive use and are not unnecessarily complicated. A phased stepwise approach is mandatory given the size of the task and the need to tune to user needs.

Ad 6.3) Delwaq will be improved with regard to the mass balance data that it produces. Post-processing tools will be developed, that facilitate the use of these data for integrated mass balance analysis and reporting. Where possible, tools should be based on new DeltaShell.

3.5 Integration in strategic R&D programmes (SO)

The proposed WQMF sub-projects described in sections 3.3 and 3.4 or parts of them should be integrated in the following existing strategic R&D programmes (SO):

1 Toolbox North Sea
2 Innovative management of water systems (Innovatieve inrichting watersystemen)
3 Diffuse emission sources (Diffuse bronnen)
4 Effects of climate on water quality and ecosystem (Effect Klimaat op wtarekwaliteit & ecosysteem)
5 Water bottom and sediment management strategies (Waterbodem en sedimentbeheers-strategieën)
6 Mitigation of soil pollution (Sanering)
7 Soil and Groundwater management strategies (Bodem en Grondwaterbeheersstrate-gieën)
8 Real time forecasting –Real time Water quality
9 Building with Nature

Such an integration would warrant that developments stay close to the knowledge questions that need to be answered. The intgeration still needs to be discussed with the project leaders involved. However, it is advocated that many of the proposed WQMF sub-projects can be allocated best to SO-programme “Development of WQMF”. These include:

1.1 Coupling of MT3D and Delwaq (generic aspects)
2.2 Design of a versatile unsaturated zone WQ model
3.1 Development of a generic processes library
3.2 Innovation of the processes library (baseline activities)
3.4 Publication of calibrations of the models
3.5 Implementation of the processes library in standardised MT3D
4.1 Parallelization of MT3D and Delwaq (generic aspects)
4.2 Improved coupling with hydrodynamics and hydrology (baseline activities)
4.3 Development of more efficient numerical solvers (baseline activities)
5.3 Uncertainty analysis (generic aspects)
5.4 Calibration and validation methodology (generic aspects)
6.1 Incorporation of innovations into standard Delwaq
6.2 Development of UIs for the WQMF
6.3 Development of tools for mass balance analysis

Below suggestions are made as to which (parts of) sub-projects could be included in each of the SO-programmes 1-9. The shared adoption of a sub-project implies the need to tune the related activities among the programmes and to join efforts as to the generic parts.

Ad 1) The project plan of SO-programme “Toolbox North Sea” acknowledges the lack of structural development of the integrated framework for hydrodynamics, water quality and ecosystem. A sub-project in 2009 concerns the development of a strategic vision on the development of “generic tools”, in which the needs for water quality and emission need to be given proper consideration. Parts of the following WQMF sub-projects could be integrated:

2.1 Generic emission module (link with river basins, see also SO-programme “Diffuse emission sources”)
3.2 Innovation of the processes library (integration of various modules, specific process

Formulations, transition fresh-saline; see also SO-programmes “Innovative management of water systems”, “Effects of climate on water quality and ecosystem”, “Water bottom and sediment management strategies” and “Mitigation of soil pollution”)
3.3 Eutrophication model calibration resulting in default coefficients (marine cases; see also SO-programme “Innovative management of water systems”)
3.4 Publication of calibrations of the models (marine cases; see also SO-programmes “Innovative management of water systems” and “Mitigation of soil pollution”)
3.6 Development of default coefficients for micro-pollutants (see also SO-programme “Water bottom and sediment management strategies”)
4.2 Improved coupling with hydrodynamics and hydrology (stability FLOW-z-layer for Delta waters; see also SO-programme “Innovative management of water systems”)
1.1 Data-assimilation for OMS WQ models (algae bloom forecasting model; see also SO-programmes “Innovative management of water systems” and “Real time forecasting”)
5.3 Uncertainty analysis (see also SO-programmes “Innovative management of water systems”, “Water bottom and sediment management strategies”, “Mitigation of soil pollution” and “Real time forecasting”)
5.4 Calibration and validation methodology (see also SO-programmes “Innovative management of water systems” and “Real time forecasting”)

Ad 2) “Innovative management of water systems” has many links to water quality , including the ecological components of the processes library. Parts of the following WQMF sub-projects could be integrated:

1.1 Coupling of MT3D and Delwaq (input from the Delwaq side; see also SO-programme “Diffuse emission sources”)
3.2 Innovation of the processes library (integration of various modules, specific process formulations; see also SO-programmes “Toolbox North Sea”, “Effects of climate on water quality and ecosystem”, “Water bottom and sediment management strategies” and “Mitigation of soil pollution”)
3.3 Eutrophication model calibration resulting in default coefficients (freshwater cases; see also SO-programme “Toolbox North Sea”)
3.4 Publication of calibrations of the models (freshwater cases; see also SO-programmes “Toolbox North Sea” and “Mitigation of soil pollution”)
4.2 Improved coupling with hydrodynamics and hydrology (stability FLOW-z-layer for reservoirs, off-line and on-line couplings; see also SO-programme “Toolbox North Sea”)
4.3 Development of more efficient numerical solvers (Delwaq)
5.1 Data-assimilation for OMS WQ models (stratification, dissolved oxygen, eutrophication; see also SO-programmes “Toolbox North Sea” and “Real time forecasting”)
5.2 Scaling over space and time for WQ models (surface water; see also SO-programmes “Diffuse emission sources” and “Water bottom and sediment management strategies”)
5.3 Uncertainty analysis (see also SO-programmes “Toolbox North Sea”, “Water bottom and sediment management strategies”, “Mitigation of soil pollution” and “Real time forecasting”)
5.4 Calibration and validation methodology (see also SO-programmes “Toolbox North Sea” and “Real time forecasting”)
6.3 Development of tools for mass balance analysis

Ad 3) “Diffuse emission sources” could take on most of the emission related aspects:

1.1 Coupling of MT3D and Delwaq (input from the MT3D side; see also SO-programme “Innovative management of water systems”)

1.2 Coupling of MT3D and ANIMO
2.1 Generic emission module (diffuse sources over and trough soil; (see also SO-programme "Toolbox North Sea")
2.2 Design of a versatile unsaturated zone WQ model (go/no-go decision)
4.1 Parallelization (MT3D; see also SO-programmes "Mitigation of soil pollution" and "Soil and Groundwater management strategies")
5.2 Scaling over space and time for WQ models (groundwater; see also SO-programme "Innovative management of water systems" and "Water bottom and sediment management strategies")

Ad 4) "Effects of climate on water quality and ecosystem" should make an inventory of processes requirements, and following this could contribute to:

3.2 Innovation of the processes library (specific process formulations; see also SO-programmes "Toolbox North Sea", "Innovative management of water systems", "Water bottom and sediment management strategies" and "Mitigation of soil pollution")

Ad 5) "Water bottom and sediment management strategies" should use Delwaq as platform. Parts of the following WQMF sub-projects could be integrated:

3.2 Innovation of the processes library (specific process formulations for active sediment and sediment-water interaction; see also SO-programmes "Toolbox North Sea", "Innovative management of water systems", "Effects of climate on water quality and ecosystem" and "Mitigation of soil pollution")
3.6 Development of default coefficients for micro-pollutants (see also SO-programme "Toolbox North Sea")
5.3 Uncertainty analysis (see also SO-programmes "Toolbox North Sea", "Innovative management of water systems", "Mitigation of soil pollution" and "Real time forecasting")

Ad 6) "Mitigation of soil pollution" should use standardised MT3D as platform. Parts of the following WQMF sub-projects could be integrated:

3.2 Innovation of the processes library (integration of chemical module, specific process formulations; see also SO-programmes "Toolbox North Sea", "Innovative management of water systems", "Water bottom and sediment management strategies" and "Effects of climate on water quality and ecosystem")
3.4 Publication of calibrations of the models (groundwater cases; see also SO-programmes "Toolbox North Sea" and "Innovative management of water systems")
3.5 Implementation of the processes library in standardised MT3D (see also SO-programme "Soil and Groundwater management strategies")
4.1 Parallelization of MT3D (see also SO-programmes "Diffuse emission sources" and "Soil and Groundwater management strategies")
5.3 Uncertainty analysis (see also SO-programmes "Toolbox North Sea", "Innovative management of water systems", "Water bottom and sediment management strategies"and "Real time forecasting")

Ad 7) "Soil and Groundwater management strategies" may have interests in the following WQMF sub-projects:

3.5 Implementation of the processes library in standardised MT3D (see also SO-programme "Mitigation of soil pollution")

4.1 Parallelization of MT3D (see also SO-programmes “Diffuse emission sources” and “Mitigation of soil pollution”)
5.2 Scaling over space and time for WQ models (see also SO-programme “Innovative management of water systems” and “Diffuse emission sources”)

Ad 8) “Real time forecasting” should take on:

5.1 Data-assimilation for OMS WQ models (generic parts; see also SO-programmes “Toolbox North Sea” and “Innovative management of water systems”)
5.3 Uncertainty analysis (generic parts; see also SO-programmes “Toolbox North Sea”, “Innovative management of water systems”, “Water bottom and sediment management strategies” and “Mitigation of soil pollution”)
5.4 Calibration and validation methodology (generic parts; see also SO-programmes “Toolbox North Sea” and “Innovative management of water systems”)

Ad 9) “Building with nature” should make an inventory of water quality processes requirements, and following this could contribute to:

3.2 Innovation of the processes library (chemical module, specific process formulations; see also other SO-programmes)

3.6 Tentative cost estimation

Table 4.1 presents an overview of roughly estimated cost. The amounts for 2009 arise from various sources. It is expected that in 2010 additional financing will result from investment plan “Wetenschapsraad”. Some additional financing may be generated within the LNI-water quality framework.

Table 4.1 Tentative estimated cost of SO-project “Development of WQMF” (kEuro).

Nr.	Sub-project	2009	2010	2011	2012
0	**Management of development WQMF**	20	20	20	20
1	**Coupling of WQ components**				
1.1	Coupling of MT3D and Delwaq (pilots not included)		50	50	?
1.2	Coupling of MT3D and ANIMO		15		
2	**Development of new WQ components**				
2.1	Generic emission module	50	40	40?	
2.2	Design of a versatile unsaturated zone WQ model			?	?
3	**Innovation and standardisation WQMF**				
3.1	Development of a generic processes library		50	25	
3.2	Innovation of the processes library		50	50	50
3.3	Eutrophication model calibration, default coefficients		30	30	?
3.4	Publication of calibrations of the models	15	20	20	20
3.5	Impl. of the processes library in standardised MT3D			40	
3.6	Dev. default coefficients for micro-pollutants				20
4	**Enhancement computational performance WQMF**				
4.1	Parallelization of MT3D and Delwaq		100	50?	?
4.2	Coupling with hydrodynamics and hydrology		30	30	30
4.3	Development of more efficient numerical solvers		10	30	30
5	**Supporting methodologies WQMF**				
5.1	Data-assimilation for OMS WQ models		75	50	?
5.2	Scaling over space and time for WQ models		40	40	?
5.3	Uncertainty analysis			20	60
5.4	Calibration and validation methodology			20	60
6	**Enhancement application efficiency WQMF**				
6.1	Incorporation of innovations into standard Delwaq		30	30	30
6.2	Development of UIs for the WQMF (dedicated)	40	50	50	
6.3	Development of tools for mass balance analysis				30
	Total	125	610	595?	350+

A Inventory of WQMF development issues

In the inventory it was pursued to identify the needs and opportunities with regard to water quality by answering the following questions:

- What is undertaken in and/or planned for the various SO/TO/SLA projects and other relevant projects of Deltares with regard to water quality in the broadest sense? (aims, activities, finances)
- What is not yet planned with regard to water quality model development and application, whereas it should be planned given the aims of the projects?
- Consequently, which are the development issues and priorities for the generic WQMF?
- Which possibilities exist to co-ordinate, combine and tune activities in the various projects that affect the development of the WQMF?
- What external developments should be taken into account?

The inventory was made by representatives of the four Deltares units involved (BGS, ZWS, ZKS, DSC), each of them taking on the relevant projects of his unit. Appendices A-D provide the "crude" findings. The inventory resulted in the issues as listed in the following sections. Quite a few of issues as identified by the units are overlapping. The issues have been regrouped and prioritised in Chapter 3.

A-1 Findings for BGS

Particularly in view of the plans concerning the development of a national framework for water quality (NHI-waterkwaliteit), the important issues in the order of priority are:

1 generic and flexible coupling of Delwaq (WAQ/ECO) to MT3D;
2 generic coupling of ANIMO to MT3D;
3 parallelization of MT3D;
4 embedding the coupled framework in UIs;
5 development of methodology for scaling over space and time;
6 development of a generic processes library for surface water and groundwater;
7 implementation of this processes library in MT3D;
8 standardisation of MT3D;
9 design study for a versatile unsaturated zone module (dependent on go/no-go decision).

NB1: The interface of MT3D and Delwaq will be at the interface of the macro-biologically active sediment layer and the deeper sediment/soil. Flexibility concerns among other things the one-way (first priority) and two-way communication between the models, and the possibility of stand-alone application. An important issue is parameterization of the effects of sediment/soil heterogeneity and tubing. Benefit needs to be taken from work that has been or will be done in projects such as "Grondwaterbijdrage kwaliteit oppervlaktewater zuidoost Brabant" and "Scaling up of sediment data to grid cell (TNO GIP)".

NB2/9: ANIMO coupling to RT3D needs to be reproduced in the standardised MT3D. Deltares need to decide if she will develop her own more versatile unsaturated zone module to replace ANIMO that is the property of Alterra. In case of a positive decision a design study will be the first step towards the development of a new module, which would have to include nutrients, organic matter, pesticides, heavy metals, salt (see proposal “Salt near root zone”, and “NHI-waterkwaliteit”). The link with Deltares’ emission module should be investigated, taking into account the GIS-based MONERIS methodology.

NB3: Parallelization of groundwater models including MT3D is urgently needed to reduce the run times of groundwater simulation. This needs to be co-ordinated with the parallelization of surface water models by DSC. A generic approach and specialist input from DSC is required.

NB4: An efficient User Interface (UI) is badly needed for setting up schematizations and model input, but also for post-processing. One should think rather of application specific UIs rather than a “standard” UI, because this is the starting point for the development of generic UI tools by DSC (DeltaShell). Also a UI with IMOD (existing UI package for MT3D) is desirable. Ideally IMOD would become part of DSC.

NB5: The scaling methodology is to facilitate both detailed local/regional model applications and river basin/national model applications. The methodology will probably affect process formulations, process coefficients and input data conversion. Available system data and computed water flows need to be pre-processed to fit spatial and temporal scales. In case of stand-alone applications of MT3D and Delwaq a scaling tool to convert MT3D results into Delwaq input by means of (de-)aggregation may be needed.

NB6/7: The generic processes library should allow for both complex and strongly simplified (parameterized) approaches. Selection can be done through option parameters. Extensions may concern “chemical equilibrium” on the basis of PhreeqC and/or CHARON. PhreeqC has been coupled to MT3DMS, but possibly a choice has to be made for reasons of maintenance efficiency and preferred functionality.
Process formulations of MT3D(MS) need to be integrated in the processes library. Priority processes can be selected from recent or ongoing projects like “Grondwaterbijdrage kwaliteit oppervlaktewater zuidoost Brabant”, SO-project “Waterbodem beheersstrategieën”, SO-project “Saneringstechnologie organische verbindingen” and PhD project “Verschoor - Metal binding DOC”. Such projects should investigate the usefulness of process formulations in the current process library. Extensions from the viewpoint of groundwater may concern the inclusion of bacterial biomass (growth, mortality, etc.).

NB8/7: The many versions of MT3DMS (multi substance), MT3D and RT3D need to be converted into one generic version, that will be the starting point for the migration of MT3D towards commercially available “Deltaris software”. MT3DMS is the preferred version, the modification of which may not take a large effort, because it is rather modular and because it contains most of the required features.

Relations with SO/TO/SLA and financing

SLA-project “NHI-waterkwaliteit” has finances in 2009 to make a design for couplings (1,2) and other development issues (5,6), and maybe to start some of these activities. A SO pre-study has been done concerning coupling MT3D-Delwaq. The incorporation of development issues into SO that can not be covered by the SLA-project has yet to be done.

Basically, finances have not been allocated yet for 1-9 for 2009 and thereafter. However, it seems reasonable to expect that 1, 2, 4 and 5 will receive at least partial funding from SLA "NHI" and SLA "Toolbox Waterkwaliteit". Possibly, SO-financing can be obtained for 2,3,6, and 8 though plan "Wetenschapsraad". Additional SO financing will be needed for 7 and 9.

A-2 Findings for ZWS

A general tendency is that current SO-, TO- and SLA-projects and other projects focus on existing model applications and offer very little opportunity for model innovation and extension. Keeping this in mind, the important issues are:

1 generic and flexible coupling of Delwaq (WAQ/ECO) to MT3D;
2 development of methodology for scaling over space and time;
3 development of a generic emission module;
4 extension and innovation of the generic processes library;
5 data-assimilation for operational management models;
6 establishment of sets of default process coefficients;
7 more efficient numerical solvers and parallelization of Delwaq;
8 improved coupling with hydrodynamics.

NB1/2: The development of the framework for "NHI-waterkwaliteit" is a spearhead for ZWS. For details, see section 3.1.

NB3: The development of the emission module has resulted in a first version. Further development is required to enhance applicability for a wide array of emission conditions and model settings. Moreover, some re-programming is required to comply with new formats of DeltaShell. The emission module should be used for "NHI-waterkwaliteit".

NB4: Relevant issues concern:

- integration of the floating nuisance algae module (BLOOM), possibly based on more detailed nutrient, detritus and extinction around the thermocline;
- limitation of phytoplankton (BLOOM) by carbon dioxide and uptake of sulphur;
- interaction of a macrophyte module with nutrients, organic matter, suspended sediments (turbidity) and light extinction;
- integration of a helophyte module (nutrients, organic matter);
- integration of grazer modules (dynamic zooplankton and benthic grazers, such as Dreissena);
- effects of artificial aeration on dissolved oxygen, carbon dioxide and methane;
- integration of CHARON for the simulation of macro-chemistry and the pH;
- the effects of macro-chemistry on the cohesiveness and erodability of sediment;
- extension of tracer options with regard to floating and settling (available in Delpar not in Delwaq);
- improvement of UITZICHT with regard to secchi depth;
- temperature .

The SO-EU projects Scenes and Wiser intend to apply water quality models for the investigation of the effects of climate change on water quality and aquatic ecosystems. The needs for modification of the processes library have not been assessed.

NB5: ZWS is preparing an extensive project on operational management for Waterboard Rivierenland. ZWS and ZKS work together on the development of OMSs for reservoirs in Singapore. Essential methodology for data-assimilation and data-assessment (decision rules) is lacking. For more details, see section 3.3.

NB6: Calibration of the various configurations of the processes library should result in well documented and published models and "default" process coefficients. Currently, SO and TO offer very little possibility to continue or start generic calibrations, to publish the results and to manage "default" coefficients. Examples are the calibrations of the eutrophication ECO-Delwaq-G model for Lake Veluwe (a shallow lake in a temperate climate), Lake Vlietzicht (deep lake in a temperate climate) and for "SDWA-Deep Lakes" (deep tropical reservoirs).
A database concerning default process coefficients for organic micropollutants (priority substances WFD) should be developed as a tool immediately accessible within Delwaq.

NB7: Given the tendency to make spatially more detailed and more comprehensive 3D Delwaq applications for large water systems requiring very short computational time steps it is urgently needed to obtain and implement more efficient numerical solvers and to parallelize Delwaq.
New numerical scheme 21 in Delwaq needs to be adjusted for 3D application, allowing for the substantial reduction of the computational burden of water quality simulations in case of strongly varying flow fields.
Parallelization of Delwaq is urgently needed to reduce the run times of 3D Delwaq simulations. This needs to be co-ordinated with the parallelization of water quantity models by DSC. A generic approach and specialist input from DSC is required.

NB8: The development of a Delft3D-WAVE/SWAN version for shallow lakes, and the coupling of this model with Delwaq is urgently needed for TO-projects concerning IJmeer/Markermeer and IJsselmeer. Such a model will allow for improved suspended sediment taking into account the effects of waves on erosion.
Moreover, because Delft3D-FLOW simulations deliver essential input for 3D water quality , too long run times (weeks) increasingly become an impediment for water quality . FLOW-z-layer and its recently implemented implicit solver needs to be improved with regard to stability.
Flow resistance in FLOW as caused by submerged vegetation may require on-line coupling with Delwaq.

A pro memori issue is the development of Delpar.

Relations with SO/TO/SLA and financing

For the situation with regard to the coupling of Delwaq and MT3D in view of SLA "NHI-waterkwaliteit", see section 3.1.

The current SO-EU-projects seem to have resources for model coupling and application only. The SO-projects "Shallow Lakes – Macrophytes (PhD)" and "Helophyte filter" have inadequate finances for the proper integration of modules into the processes library.

The “matching” SO-project “Phytoplankton Vlietland” may have resources for the integration of a module for floating nuisance algae into the processes library. There are no other finances for any of the proposed innovations of the processes library.

Within SO-project “SDWA-Deep Lakes” current finances are inadequate for continuation of the generic calibration and publishing of ECO-Delwaq-G.

The availability of little finances in 2010 and thereafter may largely inhibit the further development of the emission module.

A-3 Findings for ZKS

A general tendency is that current SO-, TO- and SLA-projects and other projects (mainly abroad) focus on existing model applications and offer very little opportunity for model innovation and extension. Keeping this in mind, the important issues are:

1 generic quantification of loads and emissions from river basins to seas;
2 extension and innovation of the generic processes library;
3 establishment of sets of default process coefficients;
4 data-assimilation for operational management models;
5 calibration, validation and uncertainty methodology;
6 more efficient numerical solvers and parallelization of Delwaq;
7 improved coupling with hydrodynamics;
8 improvement of mass balance post processing Delwaq;
9 operational coupling of Delwaq (WAQ/ECO/GEM) for fresh and saline systems.

NB1/2/3/6/7/9: The plan of SO-project “Toolbox North Sea” acknowledges the lack of structural development of the integrated framework for hydrodynamics, water quality and ecosystem. A sub-project in 2009 concerns the development of a strategic vision on the development of “generic tools”, in which the needs for water quality and emission need to be given proper consideration. One of the risks identified is the insufficient linking of indicators and transport and processes .

NB1: As a follow-on to the SO-EU-project Modelkey it is pursued to start a new EU-project (not before 2011) with regard to integrated river basin and sea for micropollutants. This project should take on the generic emission module as a basis for the quantification of land-based emissions from diffuse sources.

NB2: Relevant issues concern:

- integration of a new generic dynamic grazer module;
- integration of (suspended) sediment formulations;
- the effects of macrochemistry, microphytobenthos and zoobenthos on the cohesiveness and erodability of sediment;
- integration of a chemical module CHARON for the simulation of macro-chemistry and the pH;
- extension of fraction simulation with respect to primary emission sources;
- effects of micropollutants on primary production;
- (pm. integration of a foodweb module such as ECOPATH and a mesozooplankton-jelly fish module).

For OSPAR Delwaq has been extended with fraction simulation for secondary sources (rivers). This needs to be taken further to fractions for primary sources on land.
The SO-EU projects Dipol intends to apply water quality models for the investigation of the effects of climate change on water quality and aquatic ecosystems. The needs for modification of the processes library have not been assessed.

NB3: Calibration of the various configurations of the processes library should result in well documented and published models and "default" process coefficients. Currently, SO and TO offer very little possibility to continue generic calibrations, to publish the results and to manage "default" coefficients. An example is the calibration of eutrophication ECO-Delwaq-G model for the Wadden Sea, which is important for the TO-project "Ems-Dollard".
A database concerning default process coefficients for organic micropollutants (priority substances WFD) should be developed as a tool immediately accessible within Delwaq.

NB4/5: SO-project "Realtime WQ" (KD12.1) concerns both saline and fresh surface water systems. The fresh water sub-project deals with the development of cyanobacterial on the basis of a fuzzy logic algorithm. The saline water sub-project includes the development of data-assimilation methodology for phytoplankton and suspended sediment (also in TO-project MoS2), as well as the development of validation and uncertainty methodology.
Risk analysis for instance in relation to oil spill needs to be given attention in connection with uncertainty analysis.

The reservoir projects for Singapore urgently need the development of data-assimilation, concentration field interpolation and scaling techniques for salinity, temperature, suspended sediments, algae biomass (chlorophyll), cyanobacterial biomass, dissolved oxygen, nutrients and detritus. It is expected that operational fresh water quality will also become important in the Netherlands. Work has already been done with regard to plugging Delwaq into FEWS.
The SO/SLA/+-project "DA-Tools-OpenDA-COSTA" develops generic tools for the calibration of models (filters, etc.). Currently, no initiative has been taken yet to try and adapt these tools for Delwaq.

NB6/7: These issues are important for the TO-projects concerning the Rhine-Meuse Delta, in which there generally is little room for innovation, but also for for operational management. See also under ZWS.

NB8: Mass balances analysis is a very powerful means to check and analyze simulation results. Optimization of data produced and post-processing tools are needed to facilitate using the balance data.

NB9: The SLA-project "NHI-waterkwaliteit" also includes the estuarine and coastal waters, which requires the development of coupling tools and uniform water quality models.

Relations with SO/TO/SLA and financing

Clear visions vision are lacking from SO-, TO- and SLA-projects on the innovation of the water quality framework. These projects focus on the application of the existing framework. Consequently, no finances are available yet for most of the innovation issues.

SO-project "Toolbox North Sea" has very limited finances for the development of the integrated framework for hydrodynamics, water quality and ecosystem. According to the

current project plan developments will be restricted to hydrodynamic in 2010. This suggests that no finances will be available for water quality . However, water quality needs to be given proper attention in the strategic vision that will be developed for the project, in relation to the North Sea, the Wadden Sea and the Rhine and Meuse delta. The vision needs to be co-ordinated with the TO-projects.

Too little finances are available for the development of data-assimilation, calibration, validation and uncertainty methodologies within SO-project “Realtime WQ”.

The SO/SLA/+-project “DA-Tools-OpenDA-COSTA” will be continued the coming years. Investigating the usefulness of the available tools, the approach of the calibration of and the uncertainty analysis for Delwaq should be defined. In the next step the tools need to be adapted for Delwaq.

A-4 Findings for DSC

The following issues have been identified:

1 new user interface Delwaq;
2 core-code re-structuring Delwaq;
3 parallelization of Delwaq;
4 innovation and improvement of the processes library;
5 development of generic emission module.

NB1: A new user interface will integrate surface water models into one environment (generic, modular and flexible UI based on DeltaShell tools). Currently, the UI development and implementation focus on 1D, inclusive of Delwaq and the open processes library. ECOPLOT will be available for post-processing. Because in view of its generic structure the new UI may be rather complex, and functionality should be made more intuitive. In 2010 the attention will shift to extending the UI for 2D-3D.

NB2: Re-structuring of the core code of Delwaq is necessary for online FLOW-Delwaq applications, which would reduce the need for a separate transport solver in Delft3D and Sobek flow kernels.
Delwaq is not flexible enough with regard to the selection of substances and processes from different groups. This would have to be resolved.
There is a tendency to replace the separate morphological module of Delft3D with Delwaq. For morphological simulations in Delwaq the issue with regard to the dynamic extension of the list of sediment fractions needs to be resolved.

NB3: Work has been done on the parallelization of 3 of the 21 solvers in Delwaq. This work needs to be completed, and other solvers have to be taken on as well.

NB4: ZKS and ZWS are working on the innovation and extension of the processes library. This results in “special” applications of Delwaq for the purposes of many research and consultancy projects. Many innovations are still waiting to be integrated into the standard processes library and documentation. However, DSC leaves the initiative for this with ZKS and ZWS.

NB5: The emission module developed in co-operation with STOWA can efficiently import data from the “Emission Registration” database. Currently, it focuses on 1D Delwaq applications, but the module can be expanded for 2-3D. DSC is of the opinion that the initiative for further development is with ZWS and ZKS.

Relations with SO/TO/SLA and financing

No SO/TO/SLA budgets are available yet for “standard” Delwaq. Currently, all financing would have to come from sales revenues, which is to be shared with many other modules. Additional financing would have to be delivered by specific external projects.

A SO-project proposed for the development of “standard” Delwaq was not awarded.

A-5 Observations from the inventory

Assessing the present situation for the WQMF, the inventory resulted in the following findings:

- The development of the WQMF is poorly integrated in SO/TO/SLA. There is a tendency to rely on the existing framework, which inhibits the innovation of the WQMF and the development of new methodology.
- The principal reason for this is that strategic research needs as formulated in “SO-vraagsturing” documents relate to the ecological and water quality effects of the use of water resources and of climate change, and not so much to the tools needed for answering research questions. Another important reason is found in limited financial resources for individual projects.
- The guiding document for water related strategic research “Nationale kennis- en innovatieagenda Water 2010-2012” (SO-vraagsturing; draft 2 July 2009) contains 3 “needs” that concern the development of water quality models (A9,I11,S8) and 23 “needs” for which water quality is an important tool (A4,G9,G17,I2,I8,I9,I18, I19,I20,I25,I26,I27,I28,I29,J7,L3,M4,M6,M7,N6,Q1,P3,P4). This stipulates the need for continuous development and innovation of Deltares’ WQMF.
- Innovations of the processes library are proceeding in an incoherent way, leading to incomplete and poorly integrated modules. The migration of innovations into “standard Delwaq” will not take place when the financing problem is not resolved.
- Too little is undertaken or planned for the development of essential new water quality methodologies for data-assimilation, uncertainty analysis, risk analysis, and calibration/validation.
- Planning, co-ordination and finances have been insufficient. Consequently, a WQMF development and investment plan is urgently needed.
- Water quality needs to be given proper attention in the strategic vision that will be developed for the SO-project “Toolbox North Sea”. SO- and TO-projects concerning the North Sea, the Wadden Sea and the Rhine-Meuse Delta should be co-ordinated with regard to water quality .
- The SO-EU projects Scenes, Wiser and Dipol relate to the effects of climate change on water quality and aquatic ecosystems, and intend to apply water quality models for the investigation of the effects. A systematic review should be made by these projects to assess the adequateness of the current processes library and to identify gaps.

- SO-projects and other projects involving groundwater-surface water quality coupling need to be co-ordinated. Projects like “NHI-waterkwaliteit”, “Klimaatbestendige zoetwatervoorziening”, “Coupled groundwater/surface water flow (salination)” and “Waterbodem beheersstrategieën” should use the same building blocks for , Delwaq for surface water quality and sediment quality (macro-biologically active top layer), and MT3D for groundwater quality. This will allow for the optimal use of both financial resources and water quality expertise, which will favour the development of the WQMF as well.
- The development of the generic emission module with regard to diffuse sources of pollutants should take into account the links with unsaturated soil zone and run-off (ANIMO, MONERIS, etc.). Deltares should carry out a design study for a versatile unsaturated zone model dealing with nutrients, organic matter, pesticides, heavy metals and salt. The emission module should be used as one of the components in the framework for SLA “NHI-waterkwaliteit”.
- MT3D should be incorporated in standard Deltares software, and be provided with a user interface.
- There is a tendency in the international scientific community to share models and facilitate open source code. Deltares fails to promote its WQMF in this community by means of scientific publication, and making available well calibrated generic water quality models.
- European databases containing water quality data and simulation results are being constructed (GMES, SeaDataNet, EuroGOOS, ECOOP, EMECO, etc.). It should be investigated how Deltares can make use of these databases, and if specific plug-ins need to be developed.

B Inventory of R&D under responsibility of BGS

Goal:
To make a model instrument that can predict the influence of groundwater quality on surface water quality and vice versa for real world problems within reasonable computational times.

Activities needed (in order of temporal priority):
1 make a choice which groundwater transport model code(s) are going to be used in the WQMI (probably MT3DMS) and arrange a proper maintenance system, so that all improvements to the original code can easily be incorporated into the WQMI
Activity (partly) performed within other projects: There is a proposal for parallelization of MT3DMS (decision by Wetenschapsraad Deltares); otherwise no related activities planned

2 arrange a coupling between groundwater (MT3DMS) and surface water transport codes (DELWAQ).
This coupling should be very flexible. Three desirable options are foreseen:

1. The groundwater transport code could be run stand alone with saving the fluxes to the surface water. Afterwards the surface water model is run. Due to differences in the temporal scale it could be desirable that the surface water models are run for some parts of the simulation period of the groundwater models only.
2. For each time step the groundwater and surface water models run sequentially without feedback. Fluxes between the two domains are passed without iterative calculations. The domain for which a time step is solved first does not get information of the concentration at the end of the time step in the other domain: the inward flux into that domain is based on the concentration in the other domain at the beginning of the time step.
3. Both groundwater and surface water models run at the same time and fluxes between the two domains are passed iteratively. This option has a low priority and can be incorporated on a later stage.

The models should be able to run stand alone as well.
Activity (partly) performed within other projects: No

3 speed up calculations I (High priority). For some large scale real world problems it is expected that the WQMI will give computational times that are too long. Therefore it is crucial; that a parallelization of MT3DMS is programmed.
Activity (partly) performed within other projects: 1 There is a proposal for parallelization of MT3DMS (decision by Wetenschapsraad Deltares

4 arrange the process library so that groundwater and surface water models use the same processes and process parameters. It requires a combination of the processes that are presently used in surface water and groundwater. It will include the library of DELWAQ (from surface water) and the database of PHREEQC and simplified processes programmed into MT3DMS and RT3D (from groundwater). Off course it also requires that both models perform calculations using the process library.
Activity (partly) performed within other projects: No

5 arrange a coupling with transport codes from the unsaturated zone
Activity (partly) performed within other projects: Yes, 1. Coupling ANIMO/RT3D has been performed (could be set over to MT3DMS in stead of RT3D). 2. Within NHI coupling of salt transport with Metaswap (unsaturated domain) is foreseen.

6 arrange good user interface for WQMI
Activity (partly) performed within other projects: No

7 speed up calculations II (low priority). For some large scale real world problems it is expected that the WQMI will give computational times that are too long. Therefore besides the parallelization of MT3DMS two other activities are foreseen:

1. Streamline analysis :calculate the transport in the groundwater domain using a stream line analysis and gives fluxes to a surface water model
2. Upscaling: Make upscaling tool for subsurface domain (including local drainage and overland flow) and couple that with surface water model.

Activity (partly) performed within other projects: 1 streamline approaches are on the 'kennisagenda' of BGS; 2 The upscaling is being studied by Ph.D.'s Ype van der Velde and Joachim Rozemeijr

Inventory of development issues

Overview of projects:

1 NHI kwaliteit (Bas van der Grift)
2 Coupling ANIMO/MT3D (Gijs Janssen/ Alterra)
3 Jarno parallelization of MT3D (Jarno Verkaik)
4 Inventory coupling groundwater surface water quality (David Aquilera Rodriquez)
5 Klimaatbestendige zoetwatervoorziening Nederland – Verzilting in het NHI (Joost Delsman, Gualbert Oude Essink)
6 Aquaterra/Stromon (Ruth Heerdink)
7 Upscaling sediment data / transport phenomenon (Jasper Griffioen, David Aquilera Rodriquez, Johan Valstar)
8 Demand for development of coupled groundwater surface water flow for salt and in a later stage also energy (Esther van Baaren, Gualbert Oude Essink)
9 Salt near root zone (Ph.D. Proposal at Kennis voor Klimaat) (Gualbert Oude Essink)
10 Assessment tool for water management (Ph.D. Anja Verschoor, Jos Vink)
11 PhD research Ype van der Velde
12 SO 7.3.2 Waterbodem beheersstrategieën
13 SO 7.3.2 Gezonde bodem systemen: Waterbodem beheersstrategieën (kerndomein 11.2)
14 SO 11.2.3 Saneringstechnologie organische verbindingen, deelproject Recepsan (o.a. Niels Hartog JohanValstar)

Other sources of information:
General discussion with Wim de Lange
General discussion with Joachim Rozemeijer

Project 1: NHI kwaliteit (Bas van der Grift)
Status: SLA Project 2009

Planned activities with respect to water quality modelling and their goals in 2009: Investigate how the coupling of transport models for the unsaturated zone, groundwater and surface water should be implemented for NHI kwaliteit.

Missing items: A coupled model.

Overlapping activities with development for WQMI: Clear overlap.

Possibilities for cooperation: Yes.

Other relevant issues: NHI-kwaliteit is also executed in cooperation with Alterra.

Project 2: Coupling RT3D/Animo (Gijs Janssen + Alterra)
Status: Programming is finished; pilot in SO 2009

Finalized activities with respect to water quality modelling and their goals: Coupling of the unsaturated transport and agricultural management code ANIMO for the carbon, nitrogen and phosphor cycles with RT3D.

Planned activities with respect to water quality modelling and their goals: It will be tested on a real world site.

Overlapping activities with development for WQMI: ANIMO contains reaction module which would have overlap with our planned process library.

Possibilities for cooperation: The MODFLOW/RT3D coupling could be used in the WQMI

Other relevant issues: Presently the code is coupled to RT3D in stead of MT3DMS. Changing it to MT3DMS would be possible but needs time. This coupling is based on the unsaturated groundwater fluxes from MetaSwap, data accessibility is only possible via Alterra.

Project 3: Paralleliseren van geohydrologische transportmodellen (contact person Jarno Verkaik)
Status: SO proposal in 2009, decision by Wetenschapsraad

Planned activities with respect to water quality modelling and their goals: Parallelisation of MT3DMS and later on SEAWAT.

Missing items: None.

Overlapping activities with development for WQMI: Choice for proper version of MT3D and code maintenance. This has been discussed.

Possibilities for cooperation: Use of parallel version to reduce calculation time.

Other relevant issues: Financing not sure, maybe in 2009. Project is needed for NHI.

Project 4: Inventory coupling groundwater surface water quality (o.a. David Aquilera Rodriquez)
Status: Synergy project: finalized perhaps except for final report.

Planned activities with respect to water quality modelling and their goals: Inventory made how to couple DELWAQ and MT3D and proposal for extensions of process library

Missing items: None

Overlapping activities with development for WQMI: Gives overview for implementation options of WQMI (with coupling and process database).

Possibilities for cooperation: None

Other relevant issues: Project has more or less ended, although documentation I got is not final.

Project 5: Klimaatbestendige zoetwatervoorziening Nederland – Verzilting in het NHI (Joost Delsman, Gualbert Oude Essink)
Status Project proposal for SLA project

Planned activities with respect to water quality modelling and their goals: Extension of NHI with salt modelling for Metaswap (unsaturated zone), Modflow (groundwater), Mozart (regional surface water).

Missing items: Coupling with the surface water model SOBEK/Delwaq is not foreseen.

Overlapping activities with development for WQMI: A coupling of salt transport between three domains is being designed and implemented, although based on a different surface water model. Thinking about issues of time step size in the different domains.

Possibilities for cooperation: Make use of each other experience.

Other relevant issues: NHI is expected to involve SOBEK as well, so later on coupling with Sobek will be foreseen at some later stage.

Project 6: Modellering van de grondwaterbijdrage aan de kwaliteit van het oppervlaktewatersysteem in zuidoost Brabant, Deelrapport 2 van het Aquaterra/Stromon project
Status: Project finalized

Finalized activities with respect to water quality modelling and their goals: Calculation of load from the unsaturated zone through groundwater to the surface water for nitrate, Sulphate, cadmium, cupper, nickel and zinc. No model of sediment and surface water. The processes were modeled by Hydrus (unsaturated zone) and Modflow/MT3DMS (saturated zone), relationship with pH (not explicitly modeled, but spatial distribution from field data) and pyrite oxidation has been modeled.
Also a study of the applicability of transport along stream tubes has been studied.

Missing items: No study the surface water and sediment was performed.

Overlapping activities with development for WQMI: Use for stream tube approach in order to speed up groundwater transport calculations.

Possibilities for cooperation: Use experience of stream tube approach with chemical reactions in groundwater. Put chemical reactions (including derivation of parameters from field data) in process library.

Other relevant issues: Transient effect of groundwater flow (flow to drainage tubes, small ditches) etc. is sometimes very important on load to surface water. Therefore sequential

coupled time stepping for flow and transport models may be necessary if Modflow fluxes require too much memory storage (small time steps and long simulation period are often required for these groundwater systems).

Project 7: Upscaling sediment data to grid cell (Jasper Griffioen, David Aquilera Rodriquez, Johan Valstar)
Status TNO GIP (Geological information project) project 2009

Finalized activities with respect to water quality modelling and their goals: Develop concept for upscaling relevant transport data (reactivity, conductivity) and transport processes so that effect of fine scale heterogeneity can be incorporated in transport models with larger grid cells.

Missing items: None.

Overlapping activities with development for WQMI: Long term plan, speed up calculations by upscaling fine scale processes to larger scale, so that calculation time remains reasonable.

Possibilities for cooperation: None.

Other relevant issues: None.

Project 8: Demand for development of coupled groundwater/surface water flow for salt and in a later stage also energy (Esther van Baaren, Gualbert Oude Essink)
Status: 2 proposals for Kennis voor Klimaat tender and inventory for possible projects in which it could be used

Planned activities with respect to water quality modelling and their goals: Probable foreseen activities adjacent to present projects:

- Zeeland, quantification of salt transport from groundwater to surface water.
- Zuid-Holland modelling salt load from groundwater to surface water and their fluctuations.
- Lauwersmeer, quantification of effect of surface water levels to seepage and salt load.
- Wetterskip Fryslân, quantification salt levels in groundwater and ditches due to surface level descent, climate change.
- Effect of saline Volkerak-Zoommeer on groundwater and surface water quality.
- Groundwater flow modelling at estuaries and NHI, salt infiltration in groundwater.
- Zeeland eutrification due to ammonium load of salt seepage and agriculture. Quantify these nitrogen sources and use them to predict surface water quality.
- Climate change studies, fresh water lenses (both dunes and agricultural areas), drought damage in agriculture, cooling water, salt up groundwater and surface water.

Goals of Kennis voor Klimaat proposal 1 are:

- to model groundwater - surface water interaction for salt transport on national scale and calibrate it on some cases
- couple national database of fresh/salt water profiles to national fresh/salt water model
- Goals of Kennis voor Klimaat proposal 2 are:
- to model the salt load of groundwater –to surface water interaction on a very local scale (preferential flow near ditches)
- to upscale this process to regional models
- apply scenario for climate change effects (probably coupled system)

Missing items: No coupled groundwater - surface water model for salt and energy transport exists presently. Salt flux predicted from groundwater models is incorrect when compared to monitoring. Preferential flow should probably be included in model concept (dual porosity models or so).

Overlapping activities with development for WQMI: This item needs a coupled flow and transport model; Investigate possibility of development of the same coupling of transport models for the surface water groundwater interactions as the WQMI. In this case the salt transport model should be the same as the transport models for WQMI. For groundwater this is presently not the case.

Possibilities for cooperation: Either uses the same coupling or learn from each others experiences.

Other relevant issues: The document ‘koppeling gw-ow stof by Esther van Baaren’ has been used by Menno Genseberger to make a quick scan. Until present the quick scan has not been utilized. 2 Proposals were sent to ‘Kennis voor Klimaat’ but not approved yet.

There are plans to start using SEAWAT in stead of MOCDENS3D for salt water transport. SEAWAT is based on MODFLOW and MT3DMS and there are versions with have links with PhT3D. Moreover, NHI should have a salt transport included which after building the model is planned to transfer to SEAWAT.

Project 9: Salt near root zone (PhD Proposal at Kennis voor Klimaat, Gualbert Oude Essink)
Status: Proposal to Kennis voor Klimaat

Planned activities with respect to water quality modelling and their goals: Extension of existing local scale groundwater and surface water models with unsaturated zone, shallow groundwater in order to model salt load at root zone. Model will be extended to the loss of agricultural production due to salt and/or drought issues. The goal is to model the effect of climate change on rain lenses and their crop production.

Missing items: Coupling with unsaturated zone model for flow and transport without Alterra (preferred by Gualbert).

Overlapping activities with development for WQMI: Depends if we want to incorporate Alterra software or be independent.

Possibilities for cooperation: If Deltares wants to have Alterra-independent unsaturated zone model.

Other relevant issues: Proposal submitted to Kennis voor Klimaat, not certain.

Project 10: Assessment tool for water management (Ph.D. Anja Verschoor, Jos Vink)
Status: PhD project

Planned activities with respect to water quality modelling and their goals: Study better understanding for metal binding to DOC and biotic ligands and effect on toxicity
Incorporate results into improved metal speciation in BIOCHEM.
Missing items: Exacting understand of metal binding mechanisms.

Overlapping activities with development for WQMI: Results are incorporated in BIOCHEM.

Possibilities for cooperation: Results should be incorporated in process library of WQMI.

Other relevant issues: This project is partly a PhD research of Anja Verschoor.

Project 11: PhD research Ype van der Velde
Status Ph.D research

Planned activities with respect to water quality modelling and their goals: Study the temporal effect of groundwater flow and drainage (drains, overland flow) on surface water quality
Uses (temporally changing) travel time distributions to study impact of nitrogen on surface water quality of small catchment (Hupselse beek).

Missing items: Uses own new lumped transport model

Overlapping activities with development for WQMI: Upscaling subsurface domain.

Possibilities for cooperation: Ideas of Ype may be used to upscale groundwater domain.

Other relevant issues: He has several ideas:

- To model for instance contribution from drains, overland flow and direct seepage to surface water as a first indication of water quality.
- To upscale the groundwater domain to reservoirs, including solute transport and obtain discharge relations from groundwater flow and transport model: The groundwater flow model gives discharge fluxes of the various pathways as a function of average heads. The transport model gives a response curve for uptake and degradation of the contaminant along the various pathways. The reservoir models the average head and the mass of the contaminant in the reservoirs (surface, unsaturated zone) and uptake and loss along various pathway (overland flow, drainage, deeper groundwater flow). It makes it possible to calculate the groundwater domain with small time steps (minutes to 1 hour) which is needed to model overland flow more accurately. This idea is an extension of the Roadmap.

Project 12: SO 7.3.2 Gezonde bodem systemen: Waterbodem beheersstrategieën (kerndomein 11.2)
The SO project aims to describe and quantify the transport of pollutants through water and soil. It plans to make use of models and to perform measurements. An essential step is the exchange between water and sediments.

The project plan describes 5 subjects:

- exchange of sediment particles. This subject has mainly a physical character (erosion and sedimentation of soil particles, effect on strength, permeability), but relation with the buffering system for adsorption of contaminants is mentioned
- exchange of pore water. This subject handles the processes of adsorption/desorption of contaminants, potential availability, but also extreme events. Besides normal chemical effects also the impact on strength and permeability are mentioned.
- exchange of contaminants. This subjects mainly discusses the toxicity of contaminants (ecotoxicology), but also handles speciation of metals with is relevant for water quality modelling.

- lab developments for measurements of speciation of problematic contaminants
- makes link between sediment contaminant profile and ecological risks

This SO project has only a small free budget and in 2009 only lab and field experiments will be performed. For a later stage the project plan mentions model development, but for this year there is no budget.

Overlap: For the later planned model development there is a clear overlap with the plans for the WMQI which will also model the chemical interaction with the surface water sediments. For this later stage this project may come up with additional speciation processes for the process library.

Project 13: SO 11.2.3 Saneringstechnologie organische verbindingen, deelproject Recepsan (o.a. Niels Hartog JohanValstar)
Status SO project 2009

Planned activities with respect to water quality modelling and their goals: First investigation for possibilities to use in situ remediation technique for diffusive groundwater contamination remediation. Subjects: 1) Investigate arsenic adsorption to in situ precipitated goethite around drinking water wells, 2) investigate possibility to use wood shreds as reactive barrier for nitrate contamination.

Missing items: None.

Overlapping activities with development for WQMI: None.

Possibilities for cooperation: Results (adsorption on goethite) could be incorporated in process library of WQMI.

Other relevant issues: None.

General discussion with Wim de Lange:

Missing items: Upscale mechanism of groundwater flux to surface water. In general this often has preferential flow, outflow is mainly at the banks close to surface water level and not through the bottom of the surface water.

General discussion with Joachim Rozemeijer:

Missing items: Possibility to incorporate effect of changing surface water levels to drainage patterns. It can be handled by the coupling MODFLOW SOBEK; but in general it is often done for the main surface water system and not for every drain. Possibly there should be a stream routing routine with Q-h relations for smaller surface water systems, which should adapt the stages of rivers etc. within MODFLOW. The residence time of water in the shallow (mostly unsaturated) zone and/or overland flow has a large impact of nitrate and phosphate fluxes.

C Inventory of R&D under responsibility of ZWS

Overview: Ongoing projects

SO 9.3 – Scenes (Duel)
Objectives: effects of climate change on water quality its effect on ecological development of rivers and lakes. Quantify N-emissions to surface water at EU scale and develop EU waq model for total-Nitrogen based on emission registration and hydrological model (WaterGap).

SO 9.3 – Wiser (v. Geest)
Objectives: (1) effect of climate change on changes in hydrodynamics (lakes) and effects thereof on aquatic macrophytes (2) Effectiveness of rehabilitation measures.

SO 9.3 – Forcaster (Buijsse)
FORECASTER: Facilitating the application of Output from REsearch and CAse STudies on Ecological Responses to hydro-morphological degradation and rehabilitation). FORECASTER is one out of four selected and funded projects of the 1st call of IWRM NET.
Objective: ecological effects of hydro-morphological degradation and positioning hydro morphology in river rehabilitation strategies.
Analysis, measures and guidelines. No model development

SO 9.3 - Dipol (Laane en van Gils)
The impact on the coastal zone, as a sink for riverine and atmospheric contaminants, will be assessed as a final step in the river basin management process. The focus will be on changes that could be occur as a results of climate change: increasing rainfalls, rising groundwater, increase temperature, more frequent high and low river water discharges and rising sea water level.

To this end we propose to use a mathematical model of the whole North Sea (SCREMOTOX) including in detail the coastal zones. It links to the loads stemming from the river basins, which follow from a catchment based assessment (WP3,4 and 5) and other direct emissions. The model calculates the annual averaged distribution of contaminants in the water and surface sediments, it's relative contribution of different sources and an evaluation of ecotoxicological risk

Special attention will be paid in this project to:
1. the *coupling* of fresh and marine transport and contaminants models,
2. the changing estuarine *retention* due to climate change processes will be studied and modelled,
3. the relation between *increased erosion* in river basins and decrease estuarine retention during extreme conditions will be studied and modelled,
4. the *bioaccumulation* potential of contaminants in the North Sea will be studied and modelled for risk assessment,

TO LT Implementation WFD (KRW) (1200212 -Buijsse)
Development of KRW Verkenner-Chemie.

TO BOA waterkwaliteit en ecologie (1200211- ?)
No model development or application.

TO – Koelwater (Boderie)
Objectives: Optimisation of temperature model (SOBEK) by calibration of long term continuously measured field values along the Rhine and tributaries. Improvement of temperature in rivers. The work plan is nearly finished, topics to address are:
Benchmarking atmospheric exchange model with the Threetox model and evaluation of the optimal fit of available meteorological data for the heat-model (nr. stations, radiation and cloudiness, wind etc.). Furthermore specific topics are the influence of groundwater and mine water (Northrhine-Westfalia), shading of mountains and 3D phenomena at river mixing points (remote sensing data).

SO Innovative Management Freshwater System (1200217- Burger/Groot)
This four-year research program brings together many parallel research themes exploring lake hydrodynamics, water quality, ecology, monitoring and , which together will serve to provide Deltares with a strong fundamental scientific basis for providing new and innovative solutions to water management problems for shallow and deep lakes.

- Theme *Shallow lakes* and eco-hydraulics: improve the methods for inclusion of macrophytes in water quantity and water quality studies through one PhD position. Macrophytes (although filter feeders (=freshwater bivalves) are also mentioned) are the main focus through the PhD of Ellis Penning, she aims to improve the methods for inclusion of macrophytes in water quantity and water quality studies, focused especially on the acknowledgement of different functional and morphological groups of macrophytes. The conclusions of various field studies (Biebrza, Veluwemeer) and a flume experiment in Singapore (relation between plant morphology and patch density and flow patterns, drag force and roughness) should be implemented into the macrophytes module in the Delwaq process library with a focus on the relation with light climate.

- Theme *deep lakes*:

1. Support Deltares input in kind to the SDWA Upper Pierce Reservoir Program. This research will use an experimental approach in both the laboratory and field to examine and quantify a number of hydrodynamic, water quality and ecological processes under controlled and field conditions. This will be accompanied by a detailed field monitoring program to gain a better understanding of system functioning, and coupled to hydrodynamic and water quality to gain insights into specific processes leading to the improved management of lakes and reservoirs. The field program will include the establishment of in situ instrumented platforms to collect high quality and high frequency meteorological data, turbulence properties and water quality data from the lake in real time. New innovative monitoring methods will also be developed and tested in the Upper Peirce Reservoir. Not much water quality code development.
2. To examine hydrodynamic-ecological coupling in deep systems focusing primarily on Lake Vlietland through one PhD position, in particular the phytoplankton processes important for the of cyanobacteria in natural and artificially mixed systems (growth rates of non-homogenously phytoplankton (cyanobacteria) with buoyancy; importance of lake hydrodynamics in processes of scum formation, energy costs associated with scum formation, as well as effects on other phytoplankton species (shading), photo-inhibition under high light intensities be modelled). New code (D3D, Bloom, WAQ) for (buoyant) cyanobacteria biomass and surface scum formation, transport and disappearance.

- Theme development of *water quality framework*:

1. Define a long-term water quality model development plan encompassing all models within the Deltares organisation;
2. To improve the existing model code for phytoplankton production in stratified systems:
   a. To improve the model code for phytoplankton biomass and community composition simulations at the onset of stratification;
   b. To test the revised hydrodynamic model code with improved artificial mixing routines with the water quality and phytoplankton production models in Lake Vlietland to assess model performance and better understand the effects of artificial mixing processes on phytoplankton production.

3. To develop helophyte filters and riparian buffer processes within the existing water quality framework to provide tools for testing the efficiency of these management strategies to reduce nutrient loading and improve water quality.

TO-ANT (Groot, Boderie, Los ea) and BwN (Duel, Boderie, vGeest)
ANT aims to develop ecosystem models for Markermeer and IJsselmeer. Funding is available to develop the abiotic basis of the ecosystem models. The abiotic model is based on the deterministic of hydrodynamics including waves, temperature, chemistry (pH, macro chemistry), fine sediment dynamics and turbidity) and has been started in 2008 when the initial 3D dynamic fine sediment model for Markermeer was made (van Kessel et al, 2008).
There are five PhD positions involved in these two studies covering the following topics: system analysis, fish, filter feeders, silt and macrophytes.

Due tot changes in funding the ANT study relies heavily on the existing model framework of Delft3D and Habitat. No funds are available for development of (new)modules unless one of the three PhD's (fish, filter feeder and system analysis) takes the initiative (encouraged by us) to do so (using e.g. the open process library).
Within the BwN framework I expect model developments with respect to:

1. suspended matter (aquatic chemistry on silt characteristics) and sediment erosion strength (based on simple field measurements like density, size distribution etc.)
2. macrophytes module
   - The effect of turbidity on vegetation establishment and growth dynamics
   - The effect of submerged vegetation on light conditions

2.3- SLA – Toolbox Ecologie (Duel) also called "Ecotools"
a. Modellen voor habitat- en ecotoopanalyses (Haasnoot)

- HABITAT geschikt maken voor het doorrekenen van tijdseries: dynamisch script van PCRaster implementeren en aanpassen van user-interface
- Verbeteren van conversieprogramma voor omzetten van map-files van Delft3D naar bil-format
- Inbouwen van nieuwe functionaliteiten van Deltashell voor zover belangrijk voor toepassingen met HABITAT

b. Modellen voor stofstroomanalyses en algenmodellering (Los/Troost)
Project heeft als doel het opzetten van een productorganisatie voor Ontwikkeling en Operationalisering (O&O) en B&O van Delwaq applicaties GEM (zout) en DBS(zoet). De volgende aktitviteiten zijn relevant:

- (versie)beheer applicaties (mn in rijkswateren) default setting voor zoet-zout applicaties
- analyse van bestaande modellen met betrekking tot procesbeschrijvingen gericht op ontwikkeling van driehoeksmosselpopulaties in relatie tot de vraagstukken van het Markermeer
- aangeven van mogelijkheden voor “koppelingen” met bestaande modellen gericht op hydrodynamica, zwevende stof en slib en waterkwaliteit als input voor driehoeksmossel-model
- analyse van het Piscator-model en het inventariseren van wensen voor nieuwe ontwikkelingen (40 uur)

Overview: Instrument Development for WATER QUALITY

2.1 – Emission module (de Goede, Penaillo)
There are 3 related projects: b&o, development phase-3 (2009) and an open-MI project.
Emission module is available for application in in-house projects (including helpdesk). Promotion of use and coupling to water quality models required (KRW Verkenner, 2D/3D applications.
Emission module related projects (to check!):

- Rivierenland project ZWS
- Land van Maas en Waal
- Project met Delfland?
- Deltares-projects at ZWS/VEB/ZKS/?
- SLA - Toolbox Ecologie 2009 (Duel)

In 2009 the emission module will be launched in the Netherlands (course, publications). Also 50kE available for additional functionality and user friendliness.

The new 1D/2D/3D system (DeltaShell) is announced for end 2009 (at least the 1D part). As file formats have changed significantly the connection of (among others?) the emission module should be re-programmed.

2.2 –National Water Quality Model (SLA - Toolbox Waterkwaliteit - Groot)
Project proposal submitted to Segeren. Objective is a s National Water Quality model linked using SOBEK and closely linked to NHI. Funding comes from Toolbox Water Quality as NHI has not funds for this.

The instrument has focus on Dutch National/Large Regional scale and must be capable of water quality and ecology, especially effects of measures. Due to budget constraints, 2009 will focus on existing products/instruments such as STONE (further regionalisation), NutriCalc, KRW-Verkenner (in it’s role as coupling tool?).

Potential overlap with KRW-Verkenner (deltares) and Waterplanner (PBL) developments.

2.3- Modellen voor stofstroomanalyses en algenmodellering (SLA – Toolbox Ecologie Los/Troost)
Project heeft als doel het opzetten van een productorganisatie voor Ontwikkeling en Operationalisering (O&O) en B&O van Delwaq applicaties GEM (zout) en DBS(zoet). De volgende aktitviteiten zijn relevant:
-(versie)beheer applicaties (mn in rijkswateren)
-default setting voor zoet-zout applicaties
-maken en beheren van nuttige scripts (mctools)

2.4 Silt and macrophytes modules (ANT & BwN)

Due tot changes in funding the ANT study relies heavily on the existing model framework of Delft3D and Habitat. No funds are available for development of (new)modules unless one of the three PhD's (fish, filter feeder and system analysis) takes the initiative (encouraged by us) to do so (using e.g. the open process library).
Within the BwN framework I expect model developments with respect to:

1. suspended matter (aquatic chemistry on silt characteristics) and sediment erosion strength (based on simple field measurements like density, size distribution etc.)
2. macrophytes module
   - The effect of turbidity on vegetation establishment and growth dynamics
   - The effect of submerged vegetation on light conditions

2.5 Various – IMFW (Burger/Groot)

1. Inclusion of macrophytes in shallow water. Different functional and morphological groups of macrophytes are implemented into the macrophytes module in the Delwaq process library with a focus on the relation with light climate.
2. Phytoplankton processes important for the of cyanobacteria in natural and artificially mixed systems (growth rates of non-homogenously phytoplankton (cyanobacteria) with buoyancy; importance of lake hydrodynamics in processes of scum formation, energy costs associated with scum formation, as well as effects on other phytoplankton species (shading), photo-inhibition under high light intensities be modelled). New code (D3D, Bloom, WAQ) for (buoyant) cyanobacteria biomass and surface scum formation, transport and disappearance.
3. To improve the existing model code for phytoplankton production in stratified systems at the onset of stratification and to couple Delwaq to the revised hydrodynamic model code with improved artificial mixing routines
4. To develop helophyte filters and riparian buffer processes within the existing water quality framework to provide tools for testing the efficiency of these management strategies to reduce nutrient loading and improve water quality. aspects are nutrient uptake, silt removal and shore erosion protection..

Project experience, requirements

During several projects in the shallow lakes of lake IJsselmeer Area (IJssel-, Marker-, IJ-, Gooi- and Eemmeer) over the last one year we identified the following model improvements as essential for efficient project execution:

- simulation time of SWAN (wave model) is too long. Menno Genseberger takes the initiative for development of a SWAN version for shallow lakes (SWAN light?);
- coupling of SWAN to Delft3D using z-layers is not functional;
- make it more easy (less troublesome, more user friendly, robust) to develop a detailed sub-model of a part of an existing larger scale model (domain-decomposition).

Genserberger, Boderie en vd Wal have compose a separate memo on these issues separately for MT Kennis.

Often ecology and water quality experts are asked to give expert advise on the ecological effects of hydrological measures. Lately e.g. constructions (dams, islands) in the Markermeer but previously also e.g. artificial mixing in lakes. Tracer studies (fractie-sommen) are a very helpful tool that in fact 'visualise' the effect that hydrodynamics has on substances dissolved in water. There is a need to extend the 'tracer options' in delwaq, viz. floating tracers, sinking tracers, option to make simulations with multiple tracer events in time more user flexible,

residence time estimates base on tracer calculations. Studies concerned Eemmeer slibvang (boderie), 1200424_Almere_hydro_slib_II (Burger)

In Delwaq the state variables (modelled substances) have a starting value provided by the user in the initial conditions file. This file is also used to transfer the “memory” of the system from one simulation run to the connecting simulation (e.g. simulation run for the year 2000 uses the last results from the 1999 simulation). Such a mechanism is not available for (non-state) variables modelled in the process library. An example is the variable “the number of subsequent days a vegetation type has been submerged”. This leads to additional programming work and is sensitive to errors when running subsequent simulations. Study concerned NT2 (Smits).

Resource persons contacted:
De Goede, Meijers, Penailillo Burgos, Duel, Morales Chaves, Hulsbergen, Dionisio Pires, Groot.

Conclusions
Our commercial clients and government collaborators already expect Deltares to have highly innovative, state of the art knowledge and tools available to advice on their needs. An example of the framework for BwN and ANT is given in the in the figure below.

The fields in the yellow box are considered relevant for water quality. Given the model water quality model developments I conclude:

- (Adequate?) attention is given to:
  a. Flow/waves (see also eparate memo)
  b. Temperature/stratification (koelwater, IMFW)
  c. Suspended matter (BwN projects)
  d. Macrophytes/vegetation (BwN, IMFW)
  e. Algae (IMFW)
  f. Nutrients (Emission module)

- Not much attention is given to:
  a. sediment (chemistry and (historical) nutrient (P) release)
  b. macro-chemistry including carbon dioxide-pH (chemical sepciation/use of the same)

- Inadequate attention is given to
  a. under-water light climate

Recommendations:

- With respect to light climate. For many years the moudel UITZICHT is used. This module does not correclty describe the secchi depth (Kd, doorzicht). Thus model results are difficult to compare with field observations (including remote sensing data) Given the developments in monitoring of optical properties of surface watersw (e.g. hand held spectrometers and remote sensing) a revieuw of our software is required. Earier proposals (e.g. T2343, ontwikkeling spectrale lichtmodule) could be a starting point for this. Needless to say that under water licht climate is crucial for development of algae and macrophytes.

- Coupling of Charon-Delwaq is operational and functions for simple systems. In more complex situations (viz. Charon in combination with Bloom) it is not tested. Error messaging of Charon should be improved to make the software more user-friendly. Promotion of it's use is required.

Personal remark

It is my theory that due to artificial aeration (with air) the dissolved carbon pool in the euphotic zone is seriously lowered compared to natural conditions (Nieuwe Meer data show this). Carbon may then become limiting to algae growth. After confirming this theory our codes must be adapted, viz.

- Bloom must be extended with full nutrient dependency at least carbon (but probably also sulphur)
- D3D code for artificial re-aeration must be capable to model the effects on gas (oxygen, CO_2)

D Inventory of R&D under responsibility of ZKS

SO - Healthy water systems

The main objectives of “Toolbox North Sea” are the development of a strategic vision on how to fill research on the ecosystem health and services concept, to develop generic tools and indicators for the assessment of the aquatic ecosystem of the North Sea system, and to predict the effects of services and measures on the basis. Important side goals are the strengthening of co-operation with various scientific institutes. The North Sea system includes its river basins, and the quantification of loads is considered part of the research program.

The strategic vision is to be developed in 2009, upon which the execution of forthcoming research will start in 2010. Models for key pollutants are among the deliverables. The focus with regard to modelling for 2010 will be on hydrodynamic modelling. The Generic Ecological Model is supposed to be available in the beginning of 2009 (PhD BLOOM), the generic model for contaminants in the end of 2009 (Modelkey). One of the risks identified for the project concerns insufficient links between indicator development and transport and processes modelling.

With regard to water quality modelling in the broadest sense very little is currently explicitly included in the various sub-project plans. An active link should be established between sub-project 1 (Vision) and “Development plan WQMF”. This will bring to the attention the need to further develop the integrated generic ecosystem modelling framework especially to describe in more detail processes in estuaries and Wadden Sea with regard to nutrients, contaminants, sediment-water interaction, nutrient and carbon uptake in higher organisms zooplankton, grazers, sea grass, etc. For the North Sea also acidification due to climate change is an issue, which may require pH and CO2 modelling. Model development needs to be co-ordinated with IMARES, NIOZ and NIOO-CEMO.

Currently, there are no water quality and ecosystem modelling R&D projects for the Wadden Sea. The development of ecological and water quality modelling has come to a halt in 2007. For the continuation of the calibration and the publication of GEM/ECO-Delwaq-G no resources are currently available. It is urgently needed to resume this work because this will provide a default coefficient setting and good starting point for expected TO projects for the Wadden Sea such as the Eems-Dollard project and other shallow intertidal sea and estuary modelling. There are possibilities for co-operation in NWO-projects (3 PhDs) of NIOO-CEMO / NIOZ with regard of P-modelling in the Wadden Sea.

Current sub-projects are:

1. Project definition, phase 1 (Vethaak)
2. EU project KnowSeas (Los)
3. EU project Modelkey, contaminants (van Gils)
4. PhD project Deltares staff, eutrophication (Los)
5. PhD project Deltares staff, bioaccumulation and toxic effects (vd Heuvel)
6. Optimalisation monitoring (Laane, PhD Blauw)
7. Contaminant effects on primary production (Laane/Vethaak, guidance 2 PhDs)
8. Mesozooplankton (Langenberg, guidance PhD)

9. Strategic collaboration with IMARES (Tatman)
10. International Marine Networks ICES+LOICZ (Vethaak/Laane)
11. Development of innovative measurement methods contaminants (Smedes)
12. Project phase 2 (pm 2010-12)

Eutrophication and transboundary nutrient transports will be modeled by Deltares within sub-project 2 (KnowSeas). At this stage it is uncertain with what level of detail the Wadden Sea or the estuaries will be considered (nutrient biochemistry, sediment-water interaction), and how the organic matter component as food for higher organisms will be considered. However, in principle there are opportunities for development and application of a more advanced WQMF (see also remarks above concerning sub-project 1).

In sub-project 3 (MODELKEY), Deltares is responsible for the development of a Generic Exposure Model, which provides a rapid screening of the risk to the ecosystem of toxic pollutants stemming from individual sources of pollution or from eroding contaminated sediments. The innovation focuses on efficient forcing to cut computational burden. Although in an aggregated form, the model basically uses the fate process formulations as available in the Delwaq process library. Deltares pursues the continuation of this modelling work in a new EU-project, which should focus on integrated river basin and sea modelling. Possibilities for future innovation are found in systemizing and improving the quantification of the loads of contaminants and nutrients, especially from diffuse sources. The possibilities to link this up with the new Sobek emission module at the one hand and the use of the Moneris methodology should be investigated. There is a need for a database of micropollutant process coefficients in Delwaq. The need for upgrading process formulations is unclear. Finally, the link with ecotoxicological risk assessment should be made, possibly in connection with the “Habitat” modelling tool.

Sub-project 6 aims at optimalisation of monitoring in view of combining monitoring data with modelling. The project plan points at data-model integration (data-assimilation?) as a method but not as a product. However, we should investigate the possibilities to combine this work with work and model development for other projects consider data-assimilation in models (f.i. operational management systems modelling).

Sub-project 7 (contaminants effects) and sub-project 8 (mesozooplankton) has as such no water quality modelling components and Deltares staff is only involved by means of guidance. Nevertheless, potential spin-off of sub-project 7 includes modelling concepts for the limitation of primary production by toxicants. Implementation would require modification of the primary production module.

Sub-projects 5 (PhD), 9 (collaboration IMARIS) and 10 (International networks) and have no modelling components. Sub-project 4 (PhD) is completed.

It can be concluded that although integrated ecosystem modelling is mentioned in the project plan of Toolbox North Sea, very little is actually planned for this, and even less for water quality modelling. It is essential that the Strategic Vision will take this on.

TO – Water quality and aquatic ecology

a) TO-Eems Dollard

This project will focus in 2009 on the construction of a modelling framework for water flow, salinity, suspended sediment, dissolved oxygen and primary production. The target is to deliver adequate input into a Habitat model. It is expected that this will lead to a first inventory of needs for model innovation. The models will be applied for systems analysis and prediction in 2010-11. There may be room for some testing and calibration, but not for the model innovations as such. The Delwaq innovations may concern the interactions of microphytobenthos, phytoplankton, detritus, grazers, sediment and macro-chemistry. New sub-models may have to be (further) developed and integrated.

b) TO-Southern Rhine and Meuse Delta

The need for a generic modelling framework is unclear. The focus for the short term is with the selection of ecosystem indicators and the archivation and maintenance of extisting models.
Consequently, the needs for innovation have not been identified. However, a generic processes library, coupling and integration of marine and freshwater process formulations, a dynamic grazer module and parallelization could be among the issues.

c) TO-Western Scheldt

The existing modelling framework is being used. The need for specific innovations is unclear. Issues may be related to interactions of microphytobenthos and grazers with sediment, and to the effects of micropollutants on primary production.

Other projects concerning Water quality and aquatic ecology

a) Reservoir modelling projects

The NT2 Reservoir project and the Singapore reservoirs projects have facilitated the development and calibration of the most advanced version of our water quality modelling framework (ECO-Delwaq-G, drowned vegetation module, GHGs carbon dioxide and methane emissions). However, hardly any resources are available to participate in the research activities of the upcoming SDWA “Deep Lakes” research project (organic matter and nutrient processes in tropical reservoirs) and to publish ECO-Delwaq-G and its applications.
Moreover, the development of the water quality modelling component of OMSs is impaired greatly by the lack of development of core data-assimilation and uncertainty methodology.

b) Arabian Gulf EIA projects, Hong Kong EIA projects and Pearl river modelling

Projects will probably use the existing modelling framework. However, the quantification of emissions is usually problematic, especially with regard to diffuse sources (atmosphere, groundwater). The emission module should satisfy the specific conditions and emission quantification for these studies (1D-3D; more spatial detail in diffuse loads, coupling to groundwater models) Moreover, innovations with respect to toxicity assessments may become relevant.

c) Oil spilling risk assessments

Such projects would benefit from the development of risk and uncertainty assessment methodologies.

The interface with ecological modelling

Overview of ecological modelling issues that may be related to water quality modelling as resulting from an interview of Hans Los.

a) Ecological modelling within the process library of Delwaq

Floating nuisance algae prediction on the basis of combined fuzzy logic algorithms and deterministic modelling (SDWA Deep Lakes and SO Vlietland) although primarily driven by physical conditions may require more detailed nutrient, detritus and extinction modelling around the thermocline, no priority here as yet (contact Hans Los).

The dynamic grazer module developed by Karin van de Wolfshaar is thought to be too complex. So-called DEP models are seen as a good alternative. For further development is is necessary to make decisions on how to make a new module taking advantage of both types of models. A new module will have to be connected to the various detritus and nutrient pools. Currently, no project plans exist (contact Tineke Troost and Yenorui Morales).

The development of the water plants module seems to have been interrupted, as currently no activities are planned (contact Ellis Penning and Jan van Beek). Issues are forcing by flow velocity (FLOW), 3D modelling, contribution to light extinction, and connecting the module to the various nutrient and detritus pools.

Fish larvae are currently simulated with Delpar (contact Jan van Beek; KUDINE project with Imares). An issue is how to connect input from WAQ/ECO with regard to phytoplankton and grazers.

Currently , no plans have been formulated for the further development of an integrated marine ecosystem model on the basis of WAQ/ECO (contact Hans Los). There is a tendency to have stand-alone models for higher trophic level organisms.

b) Ecological modelling outside the process library of Delwaq

No activities are currently planned with regard to HABITAT (contact Bregje Wesenbreeg and Marjolein Haasnoot). It is yet unknown if there are specific demands for additional simulated water and sediment quality data as input into Habitat.

Ideas exist to take on ECOPATH is a MC2-type model for fish foodwebs (contact Hans Los). Possibilities to integrate it in WAQ/ECO should be investigated. An inventory should be made of the need for WAQ/ECO input. Currently, there are no plans.

The modelling of jelly fish has been considered in view of SO-project “mesozooplankton” (contact Victor Langenberg and Dick Vethaak). Currently, no plans exist. In case of the development of a WAQ/ECO module to connection to nutrients, algae and detritus would have to be made.

Findings and conclusions based on the investigated projects

- Next to nothing is foreseen with regard to the improvement and extension of water quality process formulations, let a lone the development of a generic process library.
- With regard to emission modelling only an initiative to develop a project exist.
- Nothing is foreseen with regard to modelling methodology (calibration, data-assimilation, uncertainty analysis).
- Initiatives with regard to further development of ecological models involving water quality modelling and with regard to innovation of the processes library are almost lacking.
- Links with the standard WQM software do not exist.

E Inventory of R&D under responsibility of DSC

The memo gives a brief overview of the software developments lead by DSC concerning water quality modelling. We can distinguish the following activities:

A. New user interface
B. Computational core water quality module
    a. Code restructuring
    b. Parallelization
    c. Process improvements
C. Emission module

Ad A. New user interface
The vision of DSC for surface water models is to integrate the previously separate SOBEK, DUFLOW, Delft3D and SIMONA (WAQUA/TRIWAQ) developments into one generic 0D-1D-2D-3D modelling environment (to be competitive with DHI: for both surface and ground water modelling). Features of the environment include:

- Seamless transition in 0D-1D-2D-3D modelling
- Flexible modular architecture allows for customization (same framework for quick scan analyses and detailed computations)
- Platform independent architecture (runs on Windows, Linux, …)
- Support for combination of networks, structured and unstructured meshes
- Easy access to GIS and web data resources
- Extendible environment allows for 3rd party plug-in
- Open environment allows for 3rd party software (e.g. HECRAS and MODFLOW have been coupled and run using OpenMI and visualized in the new environment)
- Supports/uses international standards (e.g. storage in CF compliant netCDF)
- Simulations can be run locally or remotely

The current implementation focuses on the generic aspects of the environment and all 1D modules; concerning water quality this includes selection of processes, specification and visualization of 1D input data, running simulations, and visualization of 1D output data. In 2010 the focus of the code development will gradually shift to 2D-3D modelling. When the simulations are run locally, the new user interface communicates in memory with the computational core (i.e. no separate input files anymore). The implementation includes support for a user-extendible open process environment similar to those available for DELWAQ and DUFLOW.

It takes a lot of effort before the new user interface satisfies all user requirements (most existing features must be transferred and while new functionality get added). One challenge is a good case analysis tool. For the time being Delft3D-WAQ users can use the ECOPLOT tool developed for ecologists.

Over the last couple of years a generic framework for data assimilation and uncertain analysis has been developed (OpenDA). This requires to some degree restructuring of the computational engine which hasn't been done for the water quality module yet (could be part of point B-a). Furthermore, the generic framework is still rather complex to use and general use of these techniques within the organization (and external consultants) will remain limited

unless the usability gets improved. It is therefore recommended to make sure that the functionality will become available in the new user interface in a more intuitive manner.

Ad B-a. Computational core water quality module – Code restructuring
Multi-disciplinary research questions lead to an increased demand in coupled simulations, e.g. online coupled flow-wave-sediment-water quality-ecology simulations to study the relation of vegetation, local and morphodynamic evolution. Over the last years DELWAQ has been modified to support online (file-based) data exchange with the SOBEK and later Delft3D flow modules. In the light of changing research questions, this implementation needs to be made more generic and faster to allow for in memory data exchange and more flexible coupling using OpenMI or similar standard interfaces. This requires restructuring of the DELWAQ input/output code down to the time loop level; some improvement is foreseen in 2009. Efficient coupling of DELWAQ to the flow module would reduce the need for a separate transport solver in Delft3D and SOBEK flow kernels.

The DELWAQ library includes a large number of processes. These processes have been bundled together into logical groups such as sediment processes, water quality processes, and ecological processes. The current implementation doesn't always allow for processes to be selected from different process groups because DELWAQ isn't able to resolve conflicts amongst a limited number of processes. This is a long-standing issue that needs to be resolved, but seems to lack momentum.

In 2006 we started implementing the morphological processes in the DELWAQ process library; however, during this implementation we encountered some limitations. In particular, DELWAQ requires that lists of species/sediment fractions are hard coded in the process library and cannot be extended dynamically based on user requirements. This is an issue that needs to be resolved before the migration of morphological processes to DELWAQ can be completed.

Ad B-b. Computational core water quality module – Parallelization
DELWAQ includes 21 solvers for different types of applications: steady-state vs dynamic, explicit vs implicit, robust vs accurate. In the first half of 2008, three explicit solvers were parallelized using MPI for distributed memory systems. There are still some issues with the scalability that haven't been addressed due to time and budget constraints, and parallelization of the other solvers is still on the to-do list. Also OpenMP parallelization on shared memory systems need to be addressed.

Ad B-c. Computational core water quality module – Process improvements
DSC does not lead any projects concerning improvements in the process formulations.

Ad C. Emission module
Developed in a cooperation of Deltares and STOWA, the emission module tracks the substances from their (local or distributed) source to the location at which they enter the open water system (the domain of our water quality modules). It allows the user to e.g. efficiently transfer data from e.g. the Dutch Emission Registration database into the water quality module based on rainfall-runoff stream paths. Although the module has been implemented to allow for extension towards 2D-3D models, it currently focuses on 1D modelling. The emission module includes features to represent substance loss due to infiltration which could be a link to ground water quality modelling.

Finance
DSC software developments are paid for using various financial resources:

1. Revenues of Delft3D and SOBEK sales
2. Budget supplied by external partners (e.g. STOWA)
3. SO budgets
4. SLA budgets

Because the 2nd – 4th budget generally come with specific development requirements, generic code developments such as user interfaces and code restructuring need to be paid for using sales revenues; however, this holds for all modules and thus the budget per module is effectively limited. STOWA contributes to the implementation of the emission module and to the renewal of the user interface (integration of DUFLOW functionality into SOBEK). DSC doesn't have any SLA budgets related to water quality modelling, and there don't seem to be any SO budgets either.

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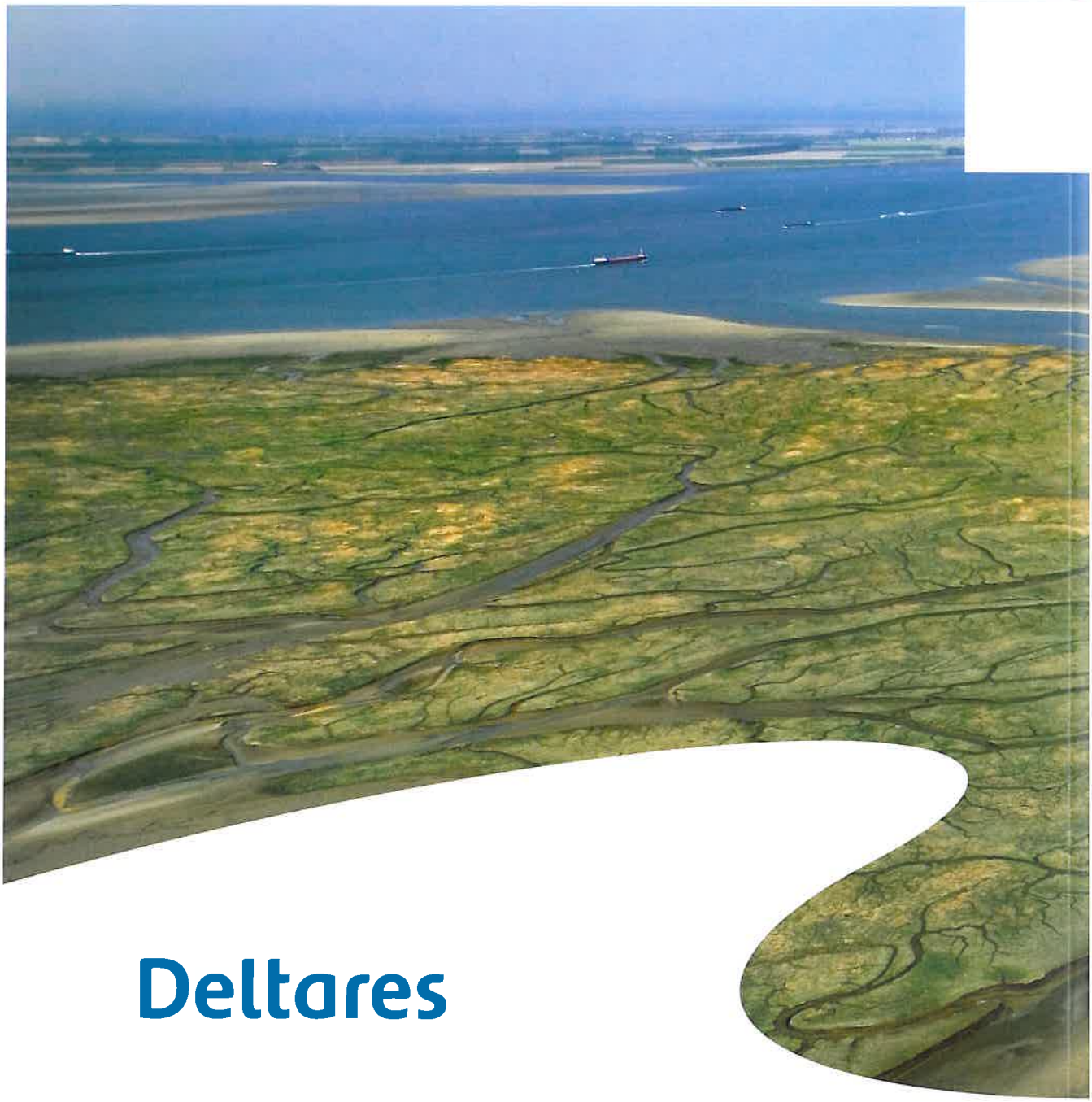

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