Waqtel UserManual

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1. Introduction

Waqtel (WAter Quality for TELemac) is a component of the Telemac-Mascaret system (TMS) which focuses on the water quality aspects. It was developed to allow the TMS's users to tackle water quality problems together with hydrodynamics.

Up to release V7P0, TELEMAC-2D and TELEMAC-3D were coupled with DELWAQ, the Deltares water quality code. This coupling, though working well for simple and medium sized models, was not suitable and cumbersome for big models. The main issue related to the use of Telemac-DELWAQ was the uncompatible parallelization of both codes.

To overcome this issue and in order to fully benefit from the parallelization effciency of the TMS, the development team introduced a first version of WAQTEL in the V7P1 release.

Waqtel is developed by the LNHE (Laboratoire National d'Hydraulique et Environnement) of the Research and Development Division of EDF (EDF-R&D). As for previous versions, the 7.1 release of the code complies with the Quality Assurance procedures of scientific and technical softwares of EDF-R&D. It is a process of construction and verification of the product quality in the different phases of his life. In particular, a software following the Quality Assurance procedures comes with a Validation Folder that describes the intended use of the software and a set of test cases. This document allows you to judge the performance and limitations of the software, situating the field of application. These tests are also used in the development of the software and are checked at every new release.

1.1 Position of the TELEMAC-3D code within the telemac modelling system

The WAQTEL software is part of the TELEMAC modelling system developed by the LNHE of EDF R&D. TELEMAC is a set of modelling tools allowing to treat every aspects of natural free surface hydraulics: currents, waves, transport of tracers and sedimentology.

WAQTEL, unlike other compnents of the TMS, can not be run in a stand-alone mode. To run a WAQTEL model, it is necessary to run TELEMAC-2D or TELEMAC-3D coupled with WAQTEL using the keyword COUPLING WITH= 'WAQTEL' (in french: COUPLAGE AVEC = 'WAQTEL')

The pre-processing and post-processing of simulations can be done either directly within the TELEMAC system or with different software that present an interface of communication with the system. We can particularly mention the following tools:

• The FUDAA-PREPRO software, developed from the FUDAA platform by the CEREMA's Recherche, Informatique et Modélisation Department, covers all the pre-processing tasks

involved by the achievement of a numerical hydraulic study, as well as a graphical post-processing tool,

- The Blue Kenue software, developed the Hydraulic Canadian Center, proposes a powerful mesh generation tool and a user-friendly post-processing tool,
- The Janet software, developed by Smile Consult GmbH, which offers among others, a mesh generation tool,
- The ParaView software, developed by Sandia National Laboratories, Los Alamos National Laboratory and Kitware, which enables to visualise 3D results, big data in particular and is open source,
- The SALOME-HYDRO software based on the SALOME platform, developed by EDF, CEA and OPENCASCADE which enables to handle raw data (bathymetry, maps, pictures, LIDAR...) until the mesh generation. The post-processing tool ParaViS available in the SALOME platform is based on the ParaView software and can visualise 1D, 2D or 3D results. A first version of SALOME-HYDRO has been available since Spring 2016,
- The QGIS software, which is an open source Geographic Information System.

1.2 Software environment

All the simulation modules are written in FORTRAN 90, with no use of the specific language extensions in a given machine. They can be run on all the PCs (or PC "clusters") under Windows and Linux operating systems as well as on the workstations under the Unix operating system.

1.3 User programming

When using a simulation module from the TELEMAC system, the user may have to program specific subroutines which are not in the code's standard release. In particular, that is made through a number of so-called « user » subroutines. These subroutines are written so that they can be modified, provided that the user has a basic knowledge in FORTRAN language, with the help of the « Guide for programming in the Telemac system » [2].

The procedure to be carried out in that case comprises the steps of:

- Recovering the standard version of the user subroutine(s) as supplied in the distribution and copying it into the current directory,
- Amending the subroutine(s) according to the model to be constructed,
- Concatenating the whole set of subroutines into a single FORTRAN file which will be compiled during the TELEMAC-2D or TELEMAC-3D launching process.

During that programming stage, the user can gain access to the various variables of the software through the FORTRAN 90 structures.

All the data structures are gathered within FORTRAN files, which are known as modules. For WAQTEL, the file name is **DECLARATION_WAQTEL.f**. To gain access to the WAQTEL data, just insert the command **USE DECLARATIONS_WAQTEL** into the beginning of the subroutine. Adding the command **USE BIEF** may also be necessary in order to reach the structure in the BIEF library.

Nearly all the arrays which are used by WAQTEL are declared in the form of a structure. For example, the access to the water depth array will be in the form H%R, %R meaning it is a

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real-typed pointer. In case of an integer-typed pointer, the % R is replaced by a % I. However, in order to avoid having to handle too many % R and % I, a number of aliases are defined, such as, the **NPOIN3**, **NELEM3** and **NPTFR2** variables. For further details, the user can refer to the programming guide in TELEMAC [2].

2. Theoretical aspects

WAQTEL offers the use of 6 water quality (WAQ) processes. These processes generate source terms that are added to the advection-diffusion equation resolved in Telemac-2d. These processes are the following:

- O2 module: which gives the evolution of oxygen O2 in the flow and accounts for the interaction with the organic load and ammoniacal load. This module is simple since it does not take into consideration all the complexity of biological phenomena linked to the production, the elimination and the transport of oxygen. For more details about this process, reader is invited to the following manual and references therein ([?]).
- Biomass module: it allows the computation of the algal biomass. It estimates the vegetal colonization as a function of several parameters such as sunshine, water temperature, ratio of renewing of water etc. This module introduces and uses 5 tracers:
 - 1. phytoplanktonic biomass (PHY)
 - 2. dissolved mineral phosphorus PO₄
 - 3. degradable phosphorus assimilated by phytoplankton (POR)
 - 4. dissolved mineral nitrogen assimilated by phytoplankton (NO₃)
 - 5. degradable nitrogen assimilated by phytoplankton (NOR)
- Eutro module: this module describes the oxygenation of a river. It is much more complex than the O₂ module since it takes into account vegetal photosynthesis and nutrients and their interactions with phytoplankton. This module introduces 8 tracers:
 - 1. phosphorus assimilated by phytoplankton (POR)
 - 2. dissolved oxygen O₂
 - 3. phytoplanktonic biomass (PHY)
 - 4. dissolved mineral phosphorus (PO₄)
 - 5. degradable dissolved mineral nitrogen assimilated by phytoplankton (NO₃)
 - 6. degradable nitrogen assimilated by phytoplankton (NOR)
 - 7. ammoniacal load (NH₄)
 - 8. organic load (L)

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These tracers are in mg/l, except biomass which is given in μ g.

• Micropol module: this module gives the evolution of micro-pollutants (radio-elements or heavy metals) in the main locations in river flows i.e. water, suspended load and bed sediments. This module introduces 5 tracers:

- 1. suspended sediments (SS)
- 2. bed sediments (BS), which are considered fix (not advected neither dispersed)
- 3. micro-pollutant species in dissolved form
- 4. part absorbed by suspended sediments
- 5. part absorbed by bed sediments
- Thermic module: this module computes the evolution of water temperature as a function of heat exchange balance with atmosphere. Only the exchanges with atmosphere are considered, those with lateral boundaries and with the bed are neglected or have to be given in the boundary conditions file.
- The Aquatic Ecodynamics library (AED2): this library is fully developed by an australian consortium (see website for more information http://aed.see.uwa.edu.au/research/models/AED/).

- [1] HERVOUET J.-M. Hydrodynamics of Free Surface Flows. Modelling with the finite element method. Wiley, 2007.
- [2] HERVOUET J.-M. Guide to programming in the telemac system version 6.0. Technical Report H-P74-2009-00801-EN, EDF R&D-LNHE, 2009.