1D/2D/3D Modelling suite for integral water solutions

Delft3D Flexible Mesh Suite

Deltares systems

DRAFT

D-Water Quality Processes Library Configuration Tool

Deltares

Enabling Delta Life

User Manual

D-Water Quality PLCT

Processes Library Configuration Tool

User Manual

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D-Water Quality PLCT, User Manual

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1 A guide to this manual

1.1 Introduction

This User Manual concerns Processes Library Configuration Tool (PLCT) of the water quality module D-Water Quality.

This module is part of several Modelling suites, released by Deltares as Deltares Systems or Dutch Delta Systems. These modelling suites are build with use of the Delta Shell framework. The framework enables to develop a range of modeling suites, each distinguished by the components and — most significantly — the (numerical) modules, which are plugged in. The modules which are compliant with the Delta Shell framework are released as D-*Name of the module*, for example: D-Flow Flexible Mesh, D-Waves, D-Water Quality, D-Real Time Control and D-Rainfall Runoff.

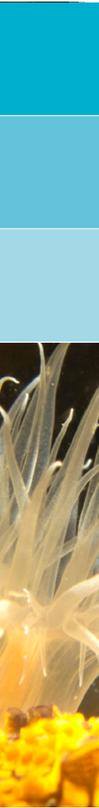Therefore, this User Manual is shipped with several modelling suites. On the *Start Page* links are provided to all relevant User Manuals (and Technical Reference Manuals) for that modelling suite. Other user manuals can be referenced. In that case, you need to open the specific user manual from the *Start Page* in the central window. Some texts are shared in different user manuals, in order to improve the readability.

1.2 Overview

Working with any simulation package requires knowledge. We distinguish three types that are required for modelling of water quality:

1 Theoretical knowledge on water quality processes in natural systems.
2 Knowledge on how to operate the Delft3D or SOBEK software tools: the Graphical User Interface, visualisation of results, etc.
3 Numerical and mathematical knowledge on modelling and the simulation package.

The level of knowledge you need, depends on what you intend to do with the water quality model. Usually there is no need to be a theoretical water quality expert, but a decent level of knowledge is required to be able to understand the rather complex interaction of processes and to assess the correctness and suitability of the result. Remember that due to numerical artefacts or inadequate input models can do predictions that are not realistic. It is up to the modeller to recognise this and to reject the simulation results. For example, a dissolved oxygen concentration of 100 mg/l should make you extremely suspicious as the normal range is 0 to 20 mg/l. If you have a suitable water quality background, D-Water Quality could be a feast of recognition for you!

Obviously, working with D-Water Quality requires you to have knowledge on how to work with the software. Basically this involves knowing which buttons to press, where to enter which input item, and how to format data to be used in the water quality modelling.

Finally, theoretical water quality knowledge has been synthesised in mathematical formulations. Additionally the flow of water and the way it transports substances through a water system makes *advection and dispersion* (i.e. transport) an essential and vital part of modelling water quality in natural systems (think of a river discharging nutrients and suspended matter into the sea). Water quality modelling in D-Water Quality involves numerically solving the so-called advection-dispersion-reaction equation. Knowledge on the principles of this equation and its implementation in D-Water Quality is necessary. Numerical skills are not required as D-Water Quality will solve the equation for you, but you should be able to recognise numerical artefacts.
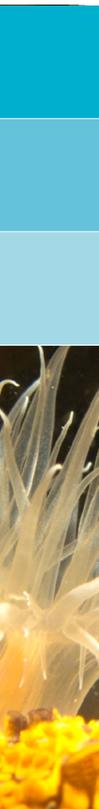
If you are not familiar with the theoretical water quality discipline, we advise you to start with the concepts on water quality modelling (**??**) and the principles of water quality (**??**) and even to study a handbook such as:

⋄ Chapra (1996)
⋄ Thomann and Mueller (1987)
⋄ Chapman (1996)
⋄ Laws (1993)

If you are a more experienced water quality modeller, the concepts in **??** are a good starting point as well and you will probably understand quickly the background of D-Water Quality.

After that, you should start with the tutorial in **??** as it will guide you through the screens and the basic functionalities of the D-Water Quality framework, without overwhelming you with a lot of details and the many possibilities and alternatives D-Water Quality contains.

The remaining chapters and appendices provide you with detailed information and can be checked whenever you need more information on a specific subject. Once you are familiar with the concepts of water quality modelling with D-Water Quality, these chapters and appendices will be your guide to further optimise your use of D-Water Quality.

1.3 Manual version and revisions

This manual applies to the D-Hydro Suite, version 2016 and later, the Delft3D Flexible Mesh Suite, version 2016 and later and the SOBEK 3.4 Suite and later.

1.4 Typographical conventions

Throughout this manual, the following conventions help you to distinguish between different elements of text.

Example	Description
Module **Project**	Title of a window or a sub-window are in given in **bold**. Sub-windows are displayed in the **Module** window and cannot be moved. Windows can be moved independently from the **Module** window, such as the **Visualisation Area** window.
Save	Item from a menu, title of a push button or the name of a user interface input field. Upon selecting this item (click or in some cases double click with the left mouse button on it) a related action will be executed; in most cases it will result in displaying some other (sub-)window. In case of an input field you are supposed to enter input data of the required format and in the required domain.
$<$\tutorial\wave\swan-curvi$>$ $<$siu.mdw$>$	Directory names, filenames, and path names are expressed between angle brackets, $<>$. For Linux environments a forward slash (/) is used instead of the backward slash (\) for Windows environments.

Example	Description
"27 08 1999"	Data to be typed by you into the input fields are displayed between double quotes. Selections of menu items, option boxes etc. are described as such: for instance 'select *Save* and go to the next window'.
delft3d-menu	Commands to be typed by you are given in the font Courier New, 10 points.
▷	In this User manual, user actions are indicated with this arrow.
[m s^{-1}] [–]	Units are given between square brackets when used next to the formulae. Leaving them out might result in misinterpretation. Most units will be in SI notation. [m AD] stands for 'meter Above Datum', which denotes a level relative to the vertical reference system in the model.

1.5 Glossary

We include here a glossary for several reasons. First, some words will occur frequently in the text and a quick reference guide could be useful. Second, in the D-Water Quality modelling terminology some words may have a slightly different meaning than you are used to. Hence it is important to realise their definition. Third, throughout the manual specific terms related to the model will be introduced. These terms are compiled here for easy reference.

Substance
A D-Water Quality state variable. D-Water Quality models the transport of active substances by solving the advection-diffusion equation numerically. The concentration of in-active substances is not affected by advective or dispersive transport. The D-Water Quality process-library contains water quality and transport processes. The concentration of active and inactive substances can be affected by water quality processes.

Active (substance)
Active substances are substances that can be transported by the flow of water, thus dissolved and particulate material in the water column.

Inactive (substance)
Inactive substances are substances that can not be transported by the flow of water. Substances that are part of the sediment are inactive substances.

Process
Processes can be divided into water quality processes and transport processes. A water quality process is associated with the transformation of substances (e.g. nitrification or mineralisation) and it generates one or more *fluxes*. A transport process is associated with the redistribution of substances and it generates one or more *velocities* or *dispersions* (e.g. sedimentation or vertical dispersive transport in a stratified water system). A process may also generate *process output*. Some processes calculate process output solely, e.g. the calculation of the extinction of light.

Process output
Fluxes, velocities and dispersions influence the concentration of specific *substances*. In case of a water quality process the calculated flux is linked to the related substance through a stoichiometric rela-

	tion.
Flux	A change of mass per unit of time and volume connected to a specific water quality *process* (for example the nitrification flux is the amount of ammonium converted to nitrate per unit of time and volume).
Segment related and exchange related information	*Process input* and *process output* is divided into segment related and exchange related information. Segment related information is known for each *segment* of the schematisation (e.g. parameters). Exchange related information is known for each *exchange area* of the schematisation (e.g. additional velocities).
Segment	Computational element of the water quality schematisation of the study area.
Exchange	The D-Water Quality model considers computational elements (or *segments*) as volumes that are linked to each other. The links or exchanges are defined by the segment number on both sides of the contact area.
Exchange area	The contact area of two linked computational elements (or *segments*).
Segment function	File (usually binary) that contains information for an input parameter that varies in time and space.
Constant	Input parameter that does not vary in time nor in space.
BLOOM	A Deltares software program to model multi-species algae growth and mortality. D-Water Quality contains an interface to BLOOM in the form of the process D40BLO.
CONSBL	A process module of the Processes Library of D-Water Quality to model grazing of phytoplankton and detritus on the basis of grazer biomass forcing.
Parameter	An input item that varies in space.
Function	An input item that varies over time.

1.6 Changes with respect to previous versions

This is the first edition which is published.

1.6.1 Processes Library Configuration Tool (PLCT)

Initially, the PLCT consists of three windows (Figure 1.1):

|		
1	**Processes Library Configuration Tool**	File managing window for opening and saving files and exiting the PLCT. The window also gives an overview of the substances selected so far.
2	**Select Groups**	Overview of available substances groups, and entry point to select substances. Also, entry point to Extra processes
3	**Messages**	Window displays messages when errors occur, mostly related to missing information.
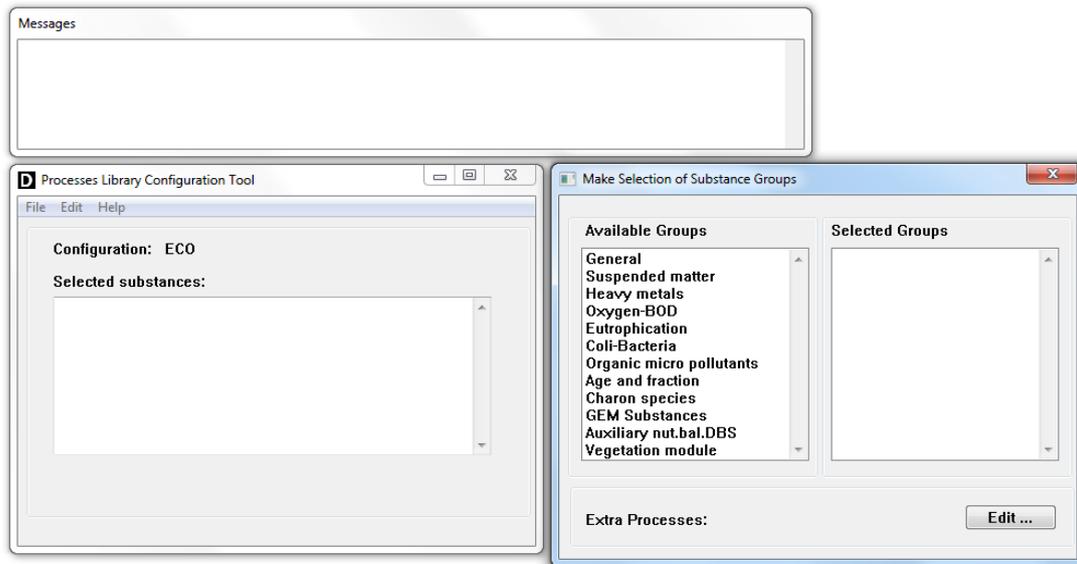
Figure 1.1: Main windows of the Processes Library Configuration Tool

The **Processes Library Configuration Tool** window displays the version number, the name of the file you are currently working on and the configuration (ECO, WAQ). Note that a $<*.0>$ and $<*.sub>$ file generated for example with the ECO configuration, can not be opened automatically in the WAQ configuration. The configuration is included in the first line of the $<*.0>$ file (for example configuration 'ECO') and can be changed manually here (e.g. configuration 'WAQ'). The PLCT will give a warning when you try to open the $<*.0>$ file.

The menu bar has the following options:

File	*New*	Start a new scenario — clear all input.
	Open...	Open an existing PLCT $<*.0>$ file.
	Save	Save the current PLCT $<*.0>$ file using the previously given name, or the default name $<substate.0>$. A substance file $<*.sub>$ is saved simultaneously.
	Save as...	Save the current PLCT $<*.0>$ file and specify its filename. A substance file $<*.sub>$ is saved simultaneously.
	Exit	Exit the PLCT.

Select groups

The **Make Selection of Substances Groups** window has three parts:

1	**Available Groups**	Shows the available substance groups within the configuration selected.
		You can select a specific group by a mouse click or standard keyboard controls. Selected substance groups will be displayed in the **Selected Groups** part on the right side of the window. Multiple groups can be selected by holding the Control key on your keyboard and selecting the second or further substance group.

|		
2	**Selected Groups**	Substance groups that are highlighted in the **Available Groups** on the left side of the window are displayed. Clicking on one of the selected substance groups here opens the **Make Selction of Substances** window, displaying the substances that are included in the substance group.
3	**Extra Processes**	Clicking *Edit. . .* opens a window with all the Extra processes that are required for the water quality processes.
		Extra Processes are processes that do not calculate a mass flux on one of the selected substances. This can be for post-processing purposes (e.g. calculating Total-Nitrogen), but lump mass fluxes as well (e.g. total resuspension).
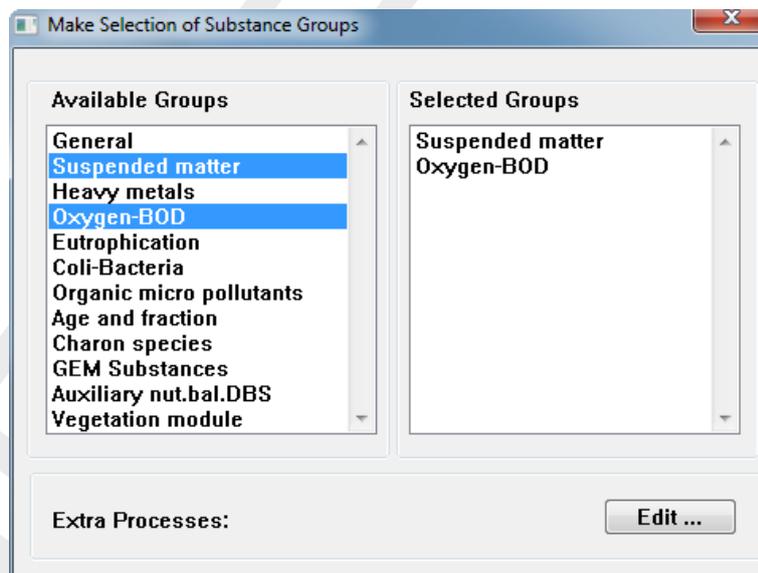
Figure 1.2: Select Groups window of the PLCT. Highlighted groups 'Suspended matter' and 'Oxygen-BOD' are selected and displayed in the right side column

Select substances

The **Make Selection of Substances** window works analogous to the **Make Selection of Substances Groups** window. Every substance group has its own **Select Substances** window. If you have selected multiple substance groups, you have to select the substances per group separately.

You can select available substances by a mouse click or standard keyboard controls. Selected substances will be displayed in the *Selected substances* part on the right side of the window. Multiple substances can be selected by holding the CTRL-key on your keyboard and selecting the second or more substance by mouse.

Clicking on one of the available substances opens the **Select Processes** window, displaying all the water quality processes that are available for this substance.

Clicking *Ready* closes the window and bring you back to the **Select Substance Group** window.
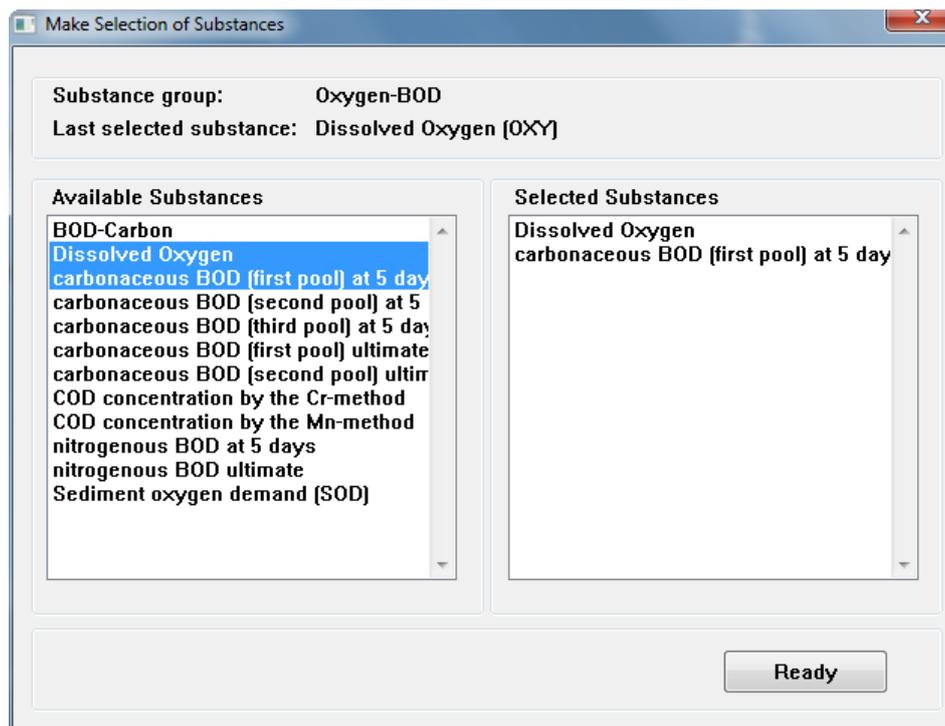
Figure 1.3: Select Substances *window for the Oxygen-BOD group. Highlighted substances 'Dissolved Oxygen' and 'Carbonaceous BOD (first pool) at 5 days' are selected and displayed in the right side column*

Select processes

The **Select Processes** window displays all processes that are available for the selected substance (Figure 1.4). You can select or 'activate' a process by checking the check box behind the process. An *Edit...* button will appear. Checking the check box once again, deactivates the process and *Edit...* will disappear. By clicking *Edit...*, you will open the **Specify Process** window (see Figure 1.5, also next section).

Occasionally, instead of the *Edit...* button, a *Define...* button will appear. A *Define...* button is displayed when the input for that specific process is not completely defined and your input is required: the **Specify Process** window will open automatically in this case. An *Edit...* button indicates that there is no missing input. There is no check on the correctness on the input, only on the completeness of the input.

After selecting and editing all required processes, you can close the **Select Processes** window by clicking *Ok*. Clicking *Cancel* will loose all changes you made since opening the window. No warning is given.

If the number of available processes is more than 12, the *Scroll Up* and *Scroll Down* buttons enable you to go through the listing of the processes.
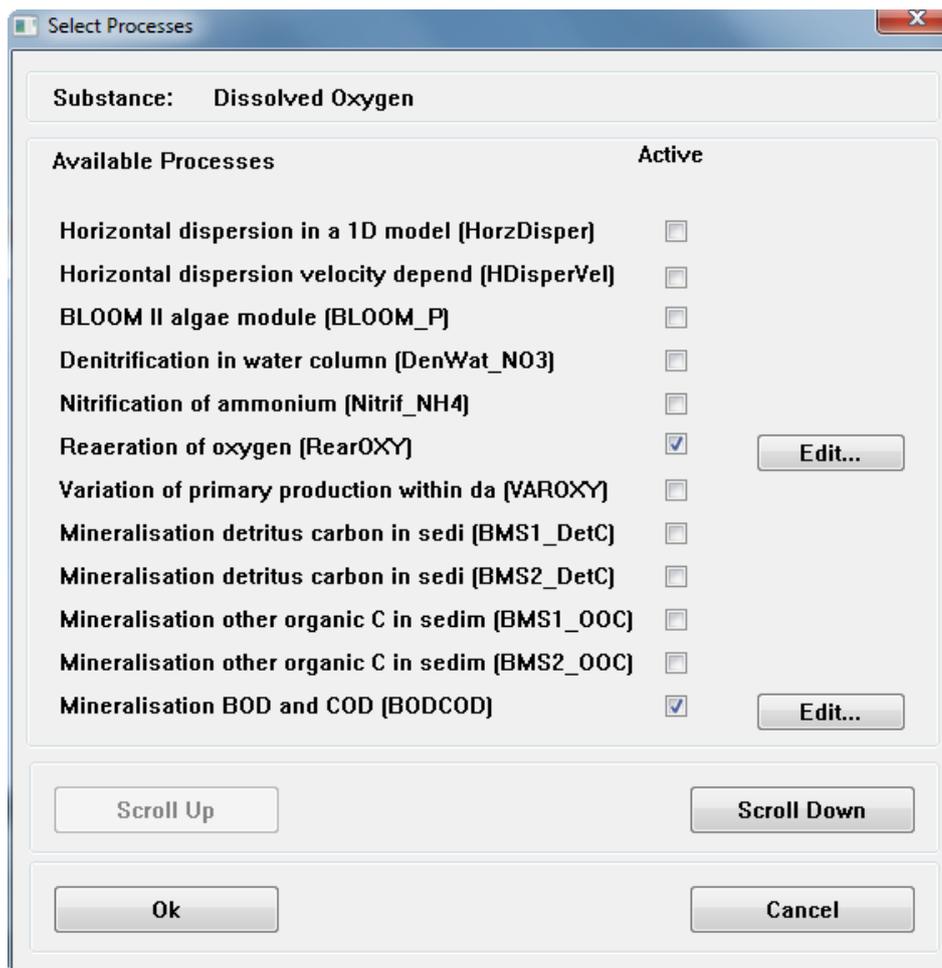
Figure 1.4: Select Processes window for 'Dissolved Oxygen'. Activated process are checked and an Edit. . . *button is shown*

Specify process

The **Specify Process** window is opened by clicking *Edit. . .* in the **Select Processes** window. The information on the **Specify Process** window is divided in six columns:

1 Description and name of the process parameter
2 Type of process parameter
   Two options:

   ◇ Constant
   ◇ Derived from another process

   A list box indicates that you have the option to make the process parameter a constant or to derive it from another process. If no list box is available, the process parameter can not be derived from another process and automatically is a constant.
3 Value of the process parameter

   ◇ When the process parameters is defined as a constant, the default value is shown. '-999' is identified as a missing value, and you will have to define a value.
   ◇ *Modelled*: the process parameter is chosen as a substance or the process parameter is available from the hydrodynamic simulation (e.g. Volume).
   ◇ Output: the process parameter is an output variable only, and no input value is required.

Figure 1.5: Specify Process window for the Reaeration of oxygen

◇ (Text string between brackets): the process parameter is derived from another process. The process name is indicated between brackets.

4 Unit
Unit of the process parameter

5 *Editable* check box
Only available for process parameters defined as Constant. Checking the Editable box will save the process parameter to the $<*.0>$ and $<*.sub>$ files. In the WAQ-GUI under *Process Parameters*, these process parameters can be given a constant value other than the default value, a time-series or a segment function. For process parameters that are not made editable the default value will be used in the water quality simulation.

6 *Output* check box
Checking the Output box will save the process parameter to the $<*.0>$ and $<*.sub>$ files as output variables. The value of the process parameter will be written to the respective output files during a water quality simulation.

After selecting and editing all required process parameters, you can close the **Specify process** window by clicking *Ok*. Clicking *Cancel* will loose all changes you made since opening the window. No warning is given.

If the number of available process parameters is more than 12, the *Scroll Up* and *Scroll Down* buttons enable you to go through the listing of the process parameters.

Each process has its own description and directives for use, see Technical Reference Manual (D-WAQ TRM, 2013).

Extra processes

Finally, after you have selected all the substance groups, the substances, their processes and the process parameters, you have to check the *Extra Processes*. The PLCT automatically accumulates all processes that do not directly calculate mass fluxes of substances. These processes are compiled in the **Specify Extra Processes** window. The window is analogous to the **Select Processes** window, with the exception that you are not allowed to deactivate processes here. If you want to deactivate an extra process, you have to go to the location in a **Specify Process** window where the process is selected. The process parameter should be changed to constant, instead of being derived from the (extra) process.

Clicking *Edit...* opens a **Specify Process** window.

Note that new extra processes can be added as well if you make such a change in a **Specify Process** window. You should check the Extra Processes list for new extra processes.

When finished you can save the PLCT file $<*.0>$ and simultaneously a substance $<*.sub>$ file will be saved. Exit the PLCT through *File → Exit*.

Substances and processes not supported by the WAQ-GUI

Substances and processes not supported by the WAQ-GUI but present in the Processes Library can be added by manual editing. Two additional user manuals are avalaible for this: D-WAQ TRM (2013) and D-WAQ Input file (2013).

References

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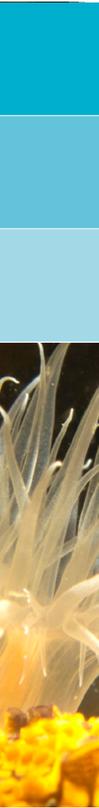
Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

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