

Mega-WATS  
Sewer process model  
User's manual  
v. 2.709



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## 1 Introduction

Mega-WATS simulates biological and chemical processes in sewer networks. It predicts how wastewater constituents are transformed and degraded as the wastewater flows from its source to the final treatment. Mega-WATS simulates all relevant processes in all parts of the network. It simulates processes in the wastewater and sewer air, predicts the amount and quality of sewer air vented to the urban atmosphere, calculates concrete corrosion, and simulates injection of chemicals to manage H<sub>2</sub>S, odor, and methane. It can simulate a tracer which is either conserved or volatile and added to either the wastewater or sewer air. Mega-WATS is, by far, the most advanced tool for modelling processes in sewers and has been validated on scores of projects ranging from small catchments to large cities with thousands of pipes.

The WATS in Mega-WATS stands for Wastewater Aerobic/Anaerobic Transformations in Sewers and represents the original sewer process model concept pioneered at Aalborg University, Denmark. The WATS concept has been developed over the last three decades of research and is continuously extended and improved as knowledge on in-sewer processes increases. It constitutes the conceptual backbone of other sewer process models on the market and has, as such, set the paradigm for sewer process modeling.

In brief, modeling with WATS typically aims at analyzing and solving sewer problems such as:

- Concrete corrosion caused by hydrogen sulfide (H<sub>2</sub>S)
- Safety hazards related to hydrogen sulfide
- Odor nuisances caused by hydrogen sulfide and VOCs being emitted into the atmosphere
- Hydrogen sulfide and VOC control strategies
- Analysis of wastewater quality at inflows to wastewater treatment plants
- Interactions between sewers and wastewater treatment plants
- Tracing illicit discharges

Key results obtained by modelling with Mega-WATS include but are not limited to:

- Mapping of H<sub>2</sub>S in sewer networks
- Mapping of concrete corrosion rates within the network
- Mapping of sewer gas releases to the atmosphere, including its content of H<sub>2</sub>S
- Assessment and quantification of all common management methods for H<sub>2</sub>S and other malodorous substances
- Identification of optimal treatment methods and locations
- Prediction of how sewer processes and addition of chemicals to the network affect the wastewater quality with respect to downstream treatment
- Assessment of future variations, for example new pipelines, climate changes, fluctuations in wastewater load and composition
- Tracing illicit discharges to the sewer, being they to the wastewater or sewer air

The largest sewer system hitherto simulated is the City of San Francisco. Its network consists of more than 31,000 pipes with a total length of 1,600 km. The simulation time for this large network is less than one minute on a decent PC.

Mega-WATS is integrated with the software Mega-Vent, which allows simulation of sewer air flow and pressure, for example, for forced ventilation studies (Section 13).

## 2 Install and run Mega-WATS

### 2.1 Hardware requirements

Mega-WATS is a 64-bit application which runs on Windows machines. If needed, it can also be delivered as a 32-bit application, which works fine, just a bit slower.

Run-times of Mega-WATS depend on the network, setup, and hardware on which it is running. For example, running a large network of 31,000 pipes, with a total length of 1670 km and 2.9 m<sup>3</sup>/s of flow on a portable work station (Lenovo with an Intel(R) Core(TM) i7-10850H CPU @ 2.70GHz, 2.71 GHz with 64 GB ram) takes 35 seconds. Smaller networks, of a thousand pipes run within a second or less.

The Mega-WATS graphical user interface (GUI) uses a main screen on which the sewer network is visualized in map view, a secondary screen for parametric visualization per downstream distance, and menus for modification of state variables and reaction kinetics, all of which, are accessible to the user. The main screen dimensions are 1510×930 pixels, and the computer screen resolution must hence be greater than these dimensions. The GUI also includes several supporting forms, which are meant to be seen together with the main screen. Hence it is helpful to use several screens of at least 1510×930 pixels or a single wide screen of 3440×1440 pixels.

Also helpful is a significant amount of RAM and a good quality graphics card with high performance and memory.

If you run Mega-WATS on poor quality computers and poor graphic cards, the forms and graphics can become distorted. Check if your forms and graphics look like the ones shown in this manual. If yes, all is well. If not, get a better computer and screens.

### 2.2 Installation

Mega-WATS does not require any installation files as it simply runs as a stand-alone executable file. Running Mega-WATS requires various input files (Section 4.2).

- Copy all input files into the same directory with the exe-file. Input files can of course also be placed in separate folders.
- Run the exe file, and the GUI will open as shown in Figure 1.
- Load the license file sent in a separate mail (\*\_MW.lic)

After having set up a network (Section 4), the network map will appear, for example as shown in Figure 2 for the city of San Francisco.

### 2.3 Placement of data files

The information on where to find the license file, the latest project loaded, as well as the Mega-Vent default directory is stored in the file General.dat which is placed in the same directory as the software. If this file is deleted, the software will ask for opening a license file next time it is opened.

Data on networks are placed in the folder where the project data is located.



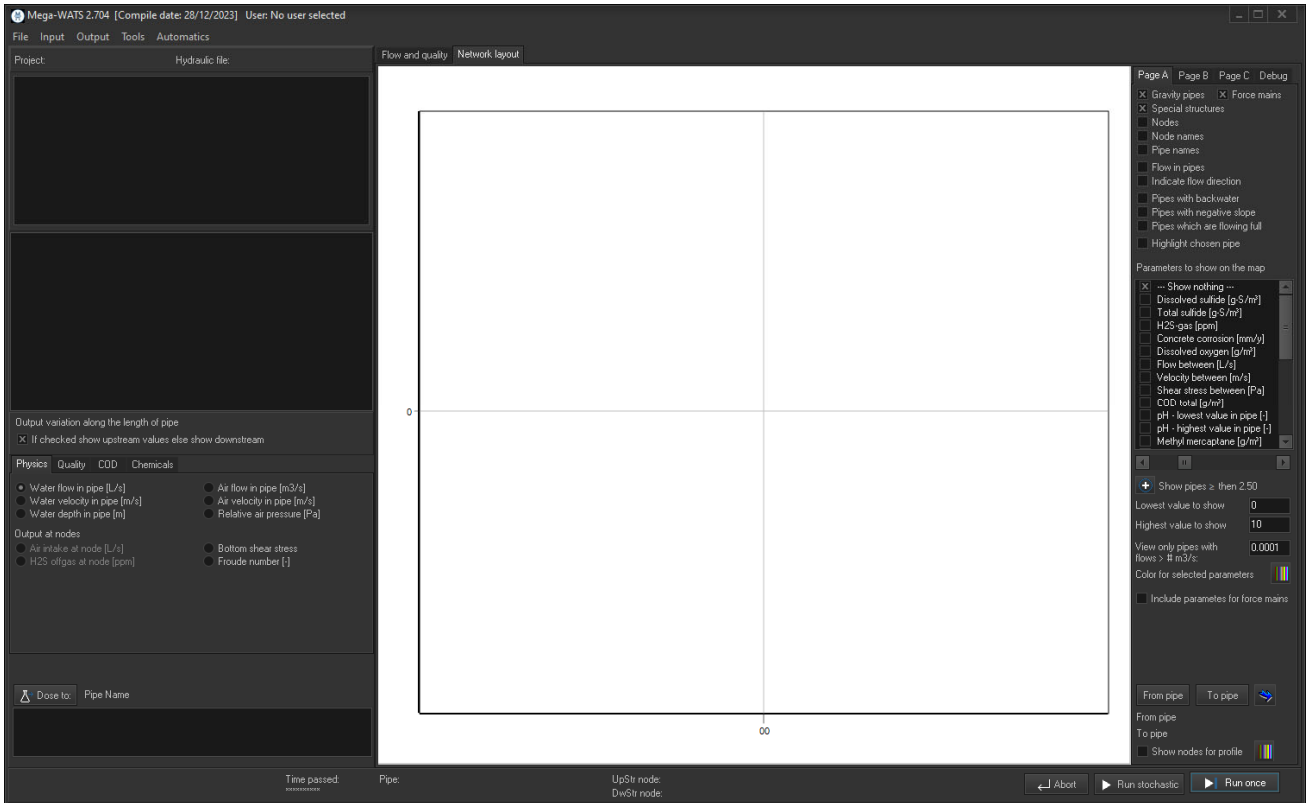


Figure 1. Mega-WATS the first time it is run. No user and no data have yet been loaded

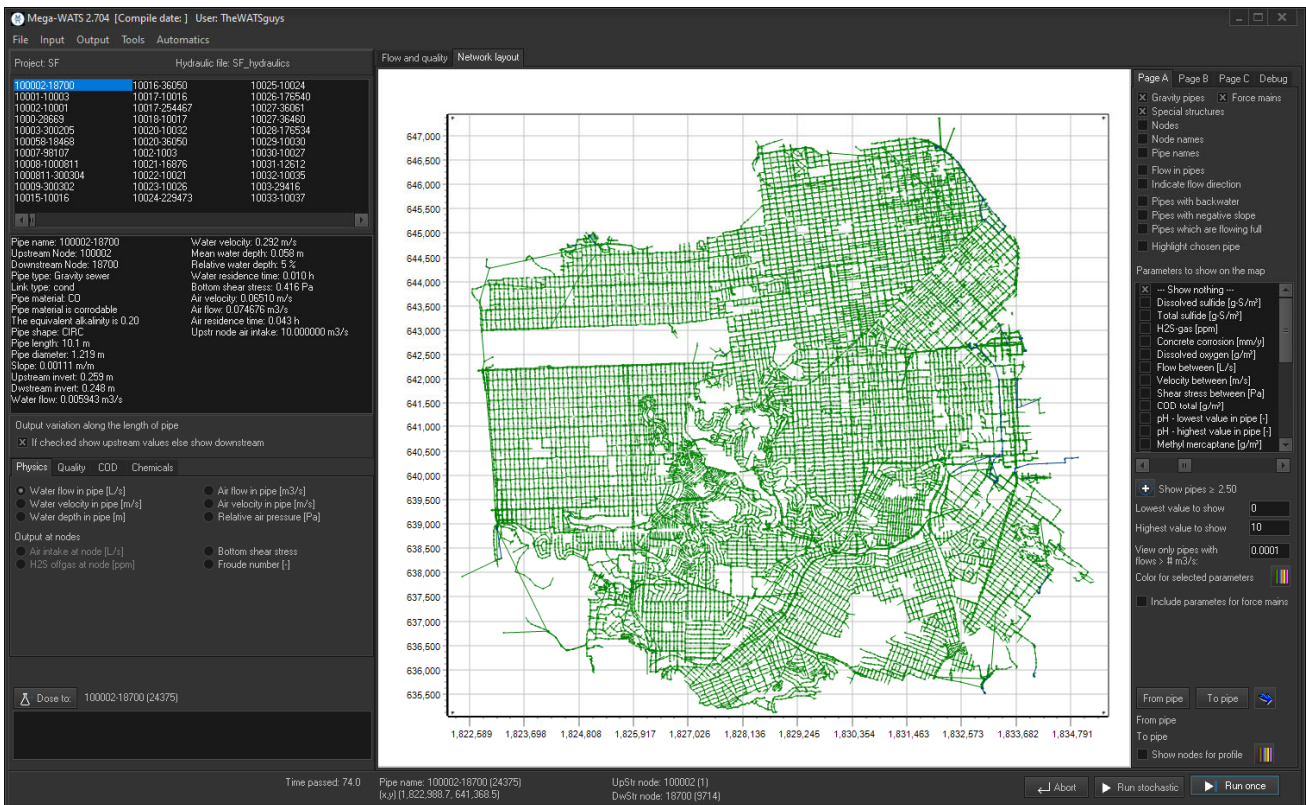


Figure 2. Mega-WATS run with a large network (San Francisco, USA)

### 3 The graphical user interface

In addition to the main visualization screen introduced above, the Mega-WATS GUI includes a secondary plot-view screen, five menus, and four pages. This allows most operations to be quickly accessible.

#### 3.1 Main menu and pages

The interface has five menu items (Figure 3): *File*, *Input*, *Output*, *Tools*, and *Automatics*.

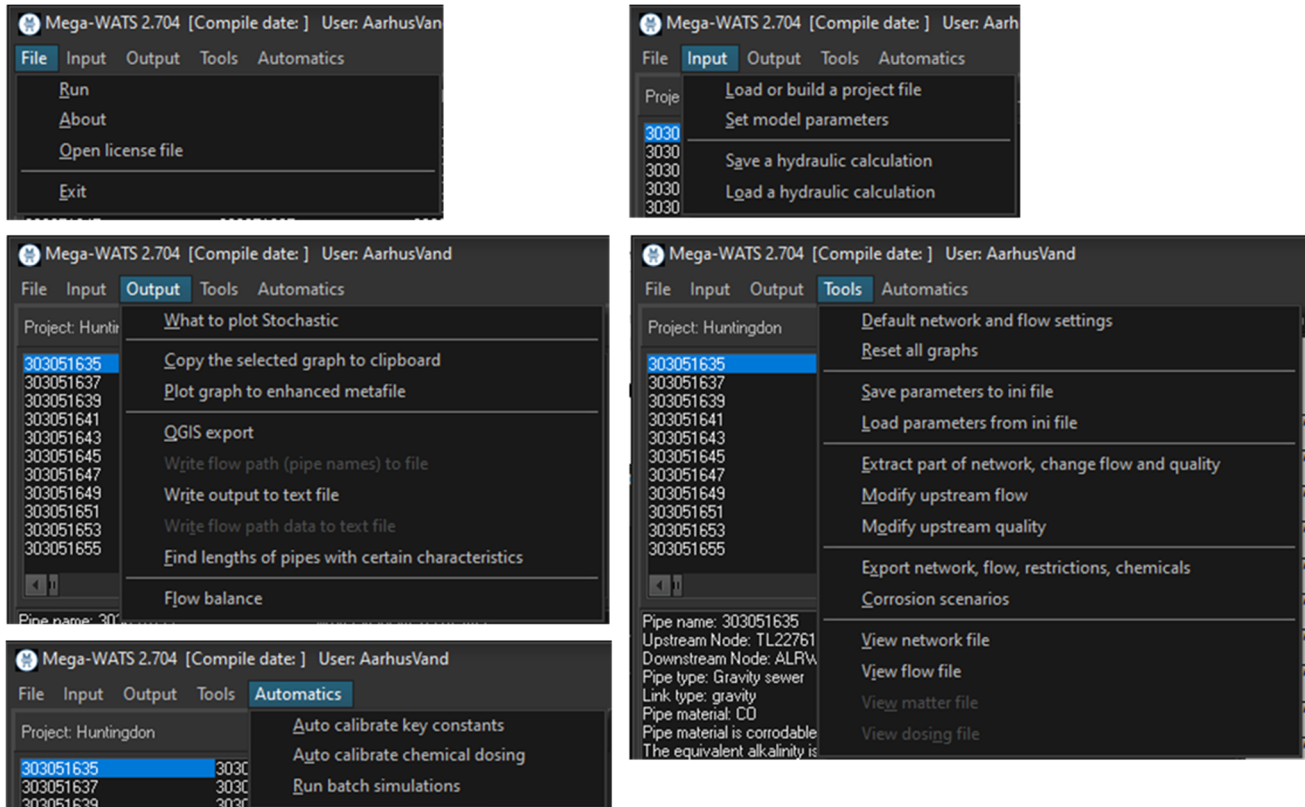


Figure 3. Menus

The pages of the GUI (Figure 4) include groups of various functions. *Page A* holds the most used functions and is the active page when starting Mega-WATS. *Pages B* and *C* hold less commonly used functions, while *Debug* is mainly used when setting up the network or modifying it in some way.

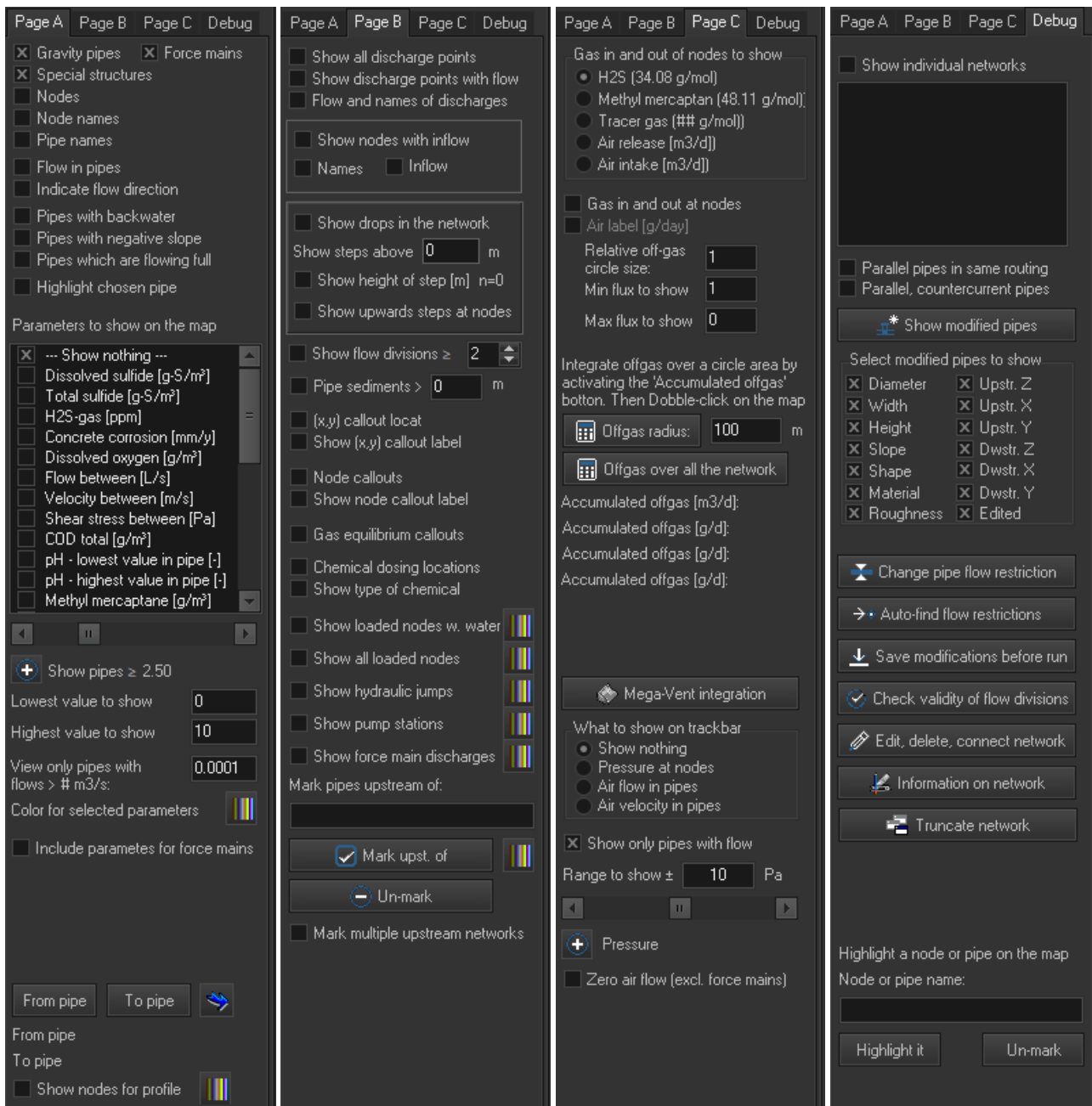


Figure 4. Pages with commands for visualization and editing. Not all license types allow access to Mega-Vent, in which case Page C looks slightly different. The same goes for methane related processes, which will affect the layout of the pages.

### 3.2 Zooming in and out

Zooming in on the map: Click on the map with the left mouse button and hold it down, drag it towards the lower right.

Zooming out goes the other way: click on the map with the left mouse button and hold it down, drag it towards the upper right (Figure 5).

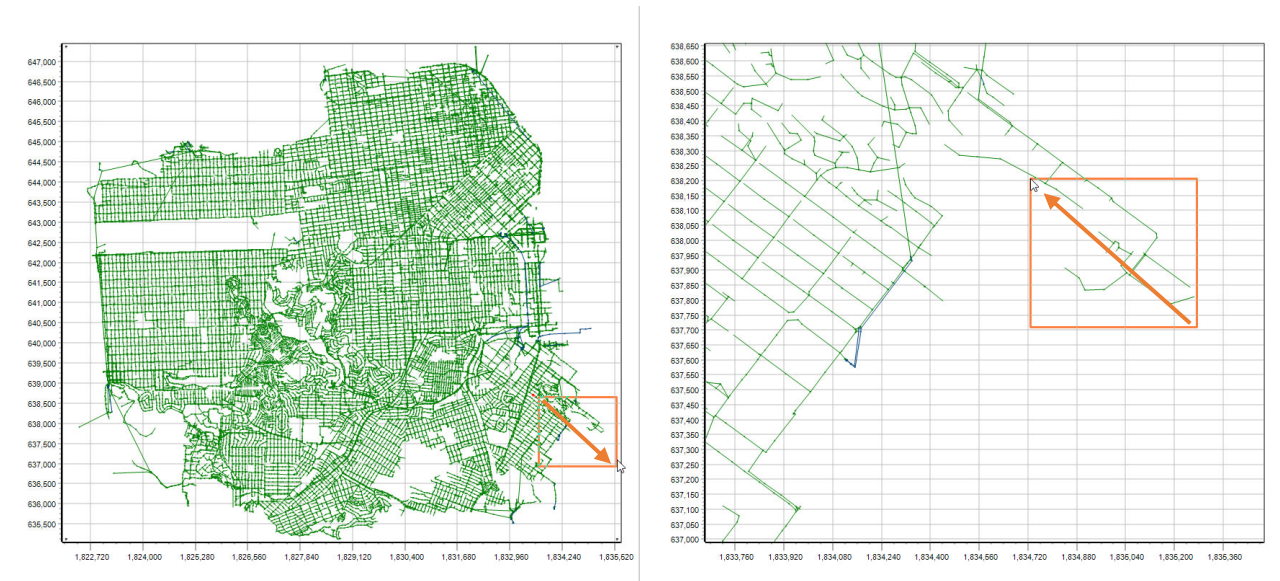


Figure 5. Zooming in and out

### 3.3 Selecting a pipe

All the pipes in the network are listed in the top left corner of the GUI. A pipe can be selected by either clicking it in the list, writing the pipe name while the list-box has focus, or double-clicking the pipe on the graphical image of the network.

When a pipe becomes selected, the list-box below is populated with various info on the pipe (Figure 6).

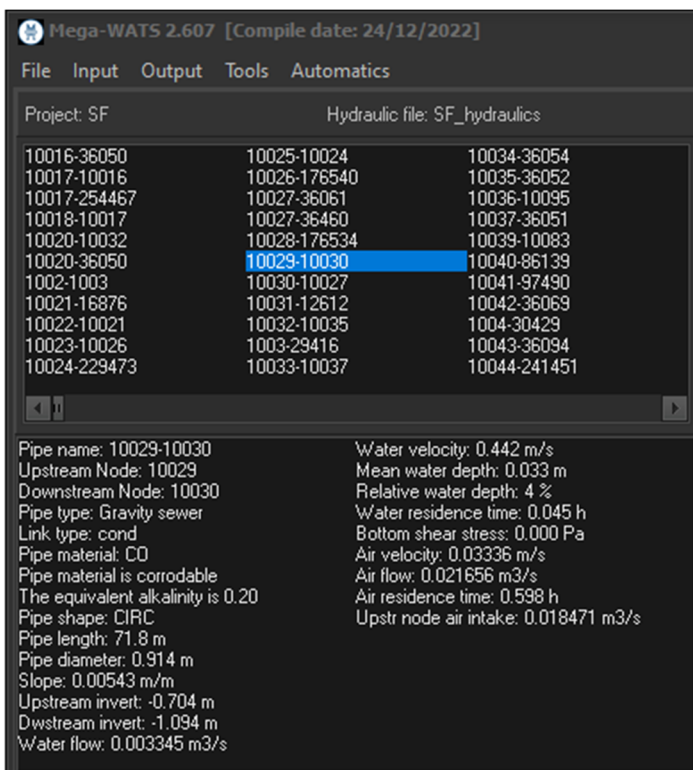


Figure 6. Pipe list-box (up) and data list-box (down) giving information on the selected pipe

### 3.4 Showing Network Map View and Parameters Plot View

Any parameter can be visualized as a function of upstream-to-downstream distance. Toggle the ‘flow and quality’ button (Figure 7) located just above the map screen to switch to plot-view. Toggle ‘network layout’ to return to map view. Upstream-to-downstream distance pertains to a user-selected flow path, and selecting flow paths is discussed later in this manual (Section 5.6).

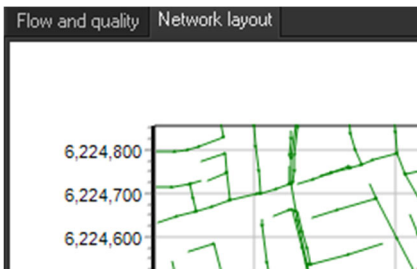


Figure 7. The main pages of Mega-WATS

### 3.5 Retrieving information from the GUI to the clipboard

It can be convenient to copy info from the GUI, for example the name of a selected pipe. This is done by selecting the relevant parameter in the list-box holding the information, right click, then copy (Figure 8).

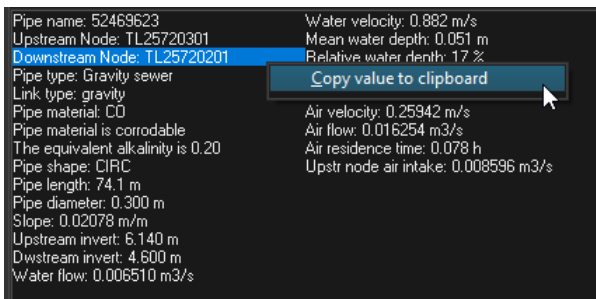


Figure 8. Copy information from the list-box holding the information on pipes.

When the coordinate on a map is needed, this can be copied by right-clicking on the map, then copying (Figure 9). This popup menu also allows copying the whole graph to clipboard.

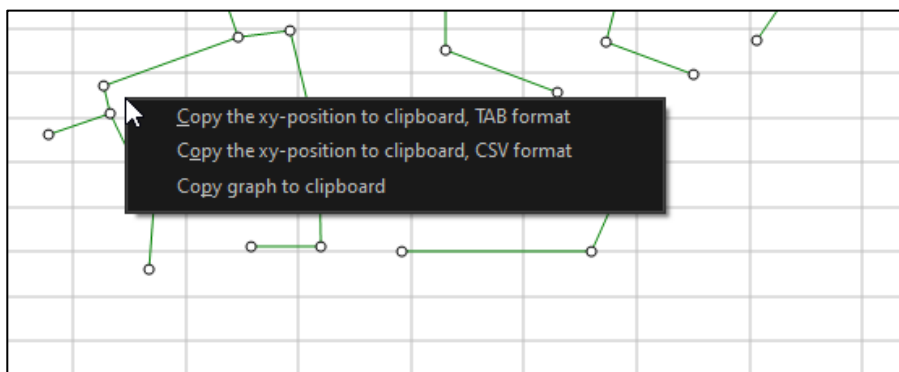


Figure 9. Copy the x,y coordinate from the map to the clipboard



Note furthermore, that various info is given below the graph, namely the name of the selected pipe and its upstream and downstream node names followed by a number in brackets. Those numbers are the pipe and node IDs used internally by Mega-WATS. The coordinate of the last click on the GUI is also shown (Figure 10).

```
Pipe name: 52468418 (503)      UpStr node: TL24727101 (2759)
(x,y) (524.836.9, 272.134.9)  DwStr node: TL24728103 (2789)
```

Figure 10. The selected pipe and its upstream and downstream node names, as well as the coordinate of the last click on the GUI.

## 4 Setting up a sewer network for simulation

In most cases the network data for Mega-WATS originates from a hydrodynamic model of some kind where the network already has been set up and hydraulically validated. While this is not a requirement for building a Mega-WATS application, it makes it easier. Data can also be drawn from an asset database. However, such data are seldom hydraulically verified, and more work must be put into validating the consistency and connectivity of the network structure.

The pipe flow in Mega-WATS is generated by applying semi-steady state non-uniform hydraulics, meaning it simulates backwater, hydraulic jumps, and such. Mega-WATS can reproduce diurnal flow patterns by linking consecutive steady state flows. The input for this can come from a hydrodynamic model in the form of either flows from connected sub-catchments or from population equivalents within such sub-catchments. It can also be generated from other sources, but that will typically require more effort than importing dry weather input values from a hydrodynamic model.

Hydrodynamic models often contain errors and inconsistencies, which may or may not cause problems for the hydrodynamic model, but which will cause problems for Mega-WATS as Mega-WATS has slightly different data requirements for the network setup. Such issues must hence be identified and removed. Tools for debugging a network are discussed in Section 5.

### 4.1 Projects

Mega-WATS is structured around the concept of a 'project'. To build a project, go to *Input -> Load or build a project* (Figure 3).

A project is built by populating the form *Build a project* (Figure 11) which is accessible from the input menu of the main form.

The first step is to *Create a new project*. Clicking the button opens a file dialog where the project file name is written. The units of the input files are defined in the input files (Section 4.2). If the units are not set correctly, Mega-WATS might crash or try to crunch numbers for a very long time without success.

*Hint: If Mega-WATS is 'hanging' in the conversion of the network file, this can be because the units have been set incorrectly. In such case one must re-start the program (ctrl-alt-del).*

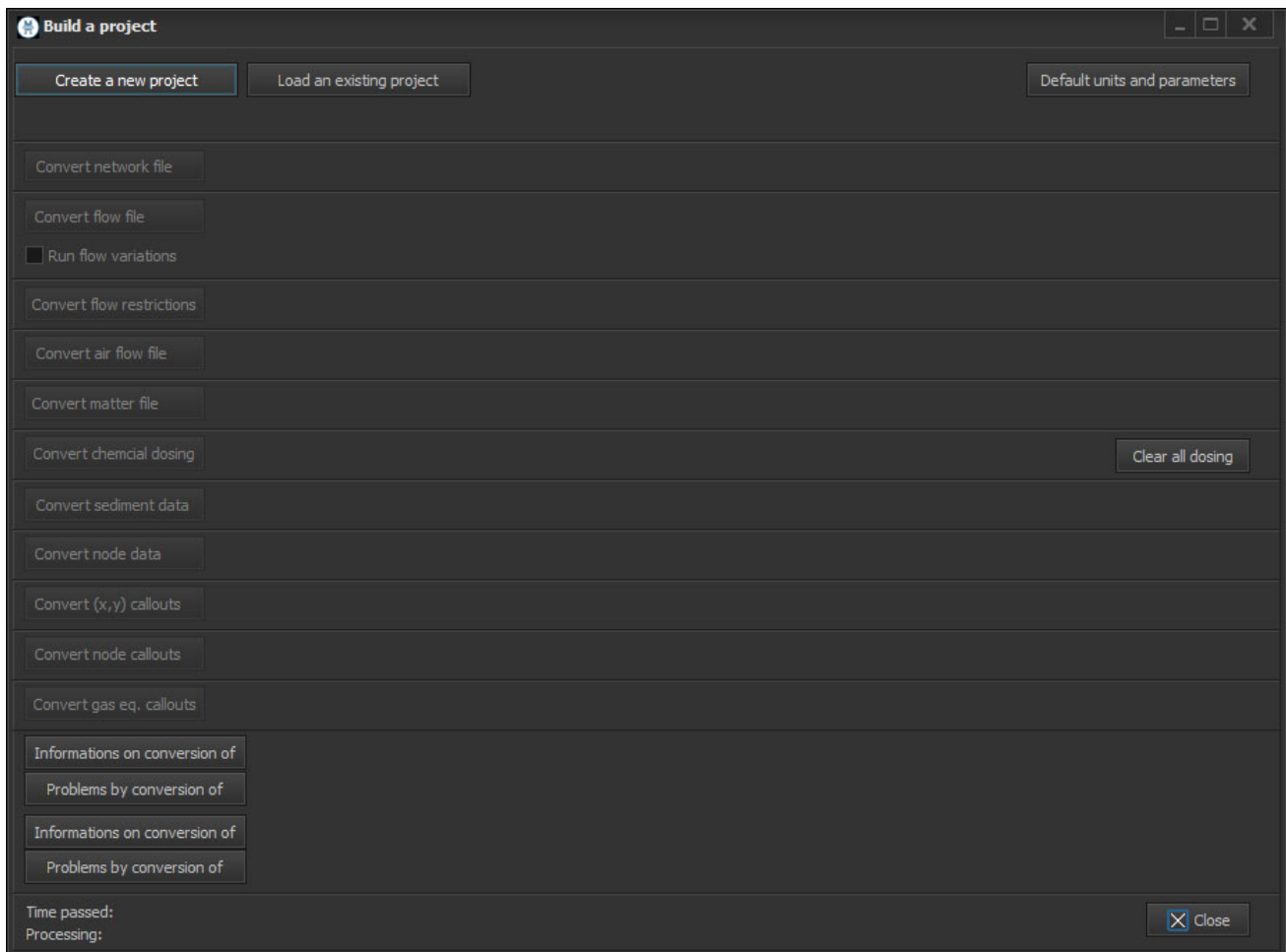


Figure 11. The form for building a project in Mega-WATS

Default units are set in the form *Set units and other parameters* (Section 4.2.12).

## 4.2 Input files

Mega-WATS data input files are text files where values are separated by the Tab character (ASCII #9). This format facilitates managing input files in a spreadsheet, which is the recommended approach. Copying any selected table of cells from a spreadsheet to a text file (i.e., a file which can be opened by simple editors such as Notepad) yields the format shown in Figure 12.

If copying from a text file to a spreadsheet, this will again put the values in the respective cells of the spreadsheet.

*Hint: It is easiest to keep all input data in a spreadsheet, where it can be edited, annotated, and tracked. To load the data into Mega-WATS, copy the desired table of cells into a text file and then load into Mega-WATS.*

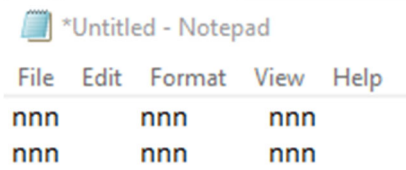


Figure 12. Text format opened in Notepad

#### 4.2.1 Network data file

The network file holds all the links and nodes of the network. The node is the identifier that associates all network data, and each node must hence be a unique identifier with a unique name. Note that Mega-WATS is case insensitive, in other words, the node 'MY\_NODE' is interpreted the same as 'my\_node'. Pipe names are also treated as unique identifiers, and in cases where a network file holds multiple pipes of the same name, Mega-WATS renames them. For example, if two pipes are named MyPipe, Mega-WATS renames them to MyPipe(1) and MyPipe(2), respectively.

The easiest way to understand the network data file, and the other data files, is by looking at the spreadsheet *Network, Flow and more example file.xlsx*

##### 4.2.1.1 The header row

The first row must hold the column headers and the second row must contain the units (Table 1). The following rows hold information on each its pipe.

The order of the columns in the network file is arbitrary and the interpretation of each column is governed by the header. It is common but not required to have the pipe identifier in the first column, then the upstream node identifier in the second column, and the downstream node identifier in the third column. While the order of columns does not matter, this structure makes it easier for the user to read the file. A header is identified by it containing a certain substring. For example, the column holding the asset name (pipe name) is defined by containing the substring 'asset' or 'muid' (case insensitive). Hence a column header indicating the pipe name could be 'Asset ID' or 'My\_asset' or 'xyzMuid777' or whatever. If it contains those substrings, it is identified as the column holding the identifier of the assets. Allowed headers are shown in Table 2.

	A	B	C	D	E	F	G	H	I
1	asset_id	us_node_id	ds_node_id	link_type	conduit_material	conduit_shape	conduit_diameter	conduit_width	conduit_height
2	Units:						in	in	in
3	119-02_139-25	119-02	139-25	Gravity	VCP	CIRC		12	12
4	119-03_119-02	119-03	119-02	Gravity	VCP	CIRC		12	12
5	119-04_119-03	119-04	119-03	Gravity	VCP	CIRC		12	12
6	119-05_119-04	119-05	119-04	Gravity	VCP	CIRC		12	12

J	K	L	M	N	O	P	Q	R	S	T
roughness	conduit_gradient	conduit_length	us_invert_z	ds_invert_z	UpLevel_C	DwLevel_C	us_node_x	us_node_y	ds_node_x	ds_node_y
Manning n	%	ft	ft	ft	ft	ft	ft	ft	ft	ft
0.013	0.069	272.3	-4.911	-5.098			6032509	2041027	6032301	2040853
0.013	0.069	160.8	-4.8	-4.911			6032634	2041130	6032509	2041027
0.013	0.139	288.7	-4.4	-4.8			6032854	2041316	6032634	2041130
0.013	0.302	364.2	-3.301	-4.4			6033133	2041548	6032854	2041316

Table 1. Network data held in a spreadsheet

Some columns are optional as indicated in Table 2.

An example of how a network file is structured is given in: *Network, Flow and more example file.xlsx* which is an addendum to this manual.

Table 2. Network file headers

Description	Must contain (case insensitive)	Required
The identifier of the link connecting two nodes, section 4.2.1.5	'asset' or 'muid'	Yes
The upstream node identifier	'us_node_id' or 'fromnode'	Yes
The downstream node identifier	'ds_node_id' or 'tonode'	Yes
The link types can be gravity mains, force mains (raising mains) and chambers (for chambers see section 4.2.1.5.4)	'link_type' or 'link type'	Yes
The material of the pipe, section 4.2.1.6	'material'	Yes
The shape of a pipe, section 4.2.1.7	'shape'	Yes
The diameter of the pipe, section 4.2.1.7	'diameter'	No
The width of the pipe, section 4.2.1.7	'width'	Yes
The height of the pipe, section 4.2.1.7	'height'	Yes
The roughness of the pipe, section 4.2.1.8	'roughness' or 'mannings' or 'eqrough'	Yes
The slope of the pipe, section 4.2.1.9	'gradient' or 'slope'	Yes
The length of the pipe	'length'	
The invert of a weirs, gates, sluice and similar, which do not have an upstream and downstream elevation, section 4.2.1.5.2	'link_invert'	No
The diameter of a weirs, gates, sluice and similar, which do not have a pipe diameter, section 4.2.1.5.2	'link_diameter'	No
The pipe upstream node (not the manhole), section 4.2.1.10	'us_invert'	Yes
The pipe downstream node (not the manhole), section 4.2.1.10	'ds_invert'	Yes
The manhole upstream node (not the pipe), section 4.2.1.10	'us_mh_invert' or 'uplevel_c'	No
The manhole downstream node (not the pipe), section 4.2.1.10	'ds_mh_invert' or 'dwlevel_c'	No
The x-coordinate of the upstream node, section 4.2.1.11	'us_node_x' or 'up_x'	Yes
The y-coordinate of the upstream node, section 4.2.1.11	'us_node_y' or 'up_y'	Yes
The x-coordinate of the downstream node, section 4.2.1.11	'ds_node_x' or 'dw_x'	Yes
The y-coordinate of the downstream node, section 4.2.1.11	'ds_node_y' or 'dw_y'	Yes
Sulfide formation rate (overrides default value), section 4.2.1.15	'k_sulfide'	No
The equivalent alkalinity of concrete (overrides default value), section 4.2.1.13	'eq_alk' or 'alk'	No
The depth of a chamber, sections 4.2.1.5.4 and 4.2.1.16	'chamber_water_depth'	No
The reaeration of a chamber, section 4.2.1.5.4	'chamber_kla'	No
Drop structure configuration, section 4.2.1.14	'drop con' or 'drop_con' or 'drop-con' or 'dropcon'	No

#### 4.2.1.2 The units row

The second row holds the units. If some other 'unit' than the listed ones are used, Mega-WATS defaults back to the default settings (section 4.2.12). While loading the data, Mega-WATS shows a warning that such unknown unit was encountered.

It is recommended to include the units as a row as this ensures that Mega-WATS always interprets the units of the columns correctly.

The row holding the units must have the first column second row including the string 'units' (case insensitive). In the example spreadsheet the form 'Units:' is used. The following cells then contain the units

of the values in the columns (Table 1). If it does not hold this string, the second row is interpreted as the first pipe in the network.

Table 2 provides the identifiers which must be used for each category of units.

Table 3. Units which can be used in the network and flow data files

Type	Unit	Identifier for unit
<b>Diameter</b>		
Width	meter (the SI-unit)	m, meter, metre
Height	centimeter (0.01 m)	cm, centimeter, centimetre
Length	millimeter (0.001 m)	mm, millimeter, millimetre
Inverts	US inches (0.0254001 m)	in, inch, inches
Elevations	US feet (0.3048 m)	ft, feet, foot
<b>Coordinates</b>		
Roughness	Equivalent sand roughness, Nikuradse sand roughness (m)	sand-m, sand-meter, sand-metre, sand m, sand meter, sand metre
	Equivalent sand roughness, Nikuradse sand roughness (mm)	sand-mm, sand-millimeter, sand-millimetre, sand mm, sand millimeter, sand millimetre
	Manning M number	Manning-M, Manning M
	Manning n number	n, Manning-n, Manning n
Gradient	Unitless (m/m)	m/m, meter/meter, metre/metre, ft/ft, foot/foot, feet/feet
	Percent (100 × m/m)	%, percent
	Per mille (1000 × m/m)	‰, permille, per mille
Alkalinity	Equivalent alkalinity (concrete)	g/g, kg/kg, g caco3/g concrete
Water flow	cubic meter per second (m3/s)	m3/s, m3 s-1
	cubic meter per hour (m3/h)	m3/h, m3 h-1
	cubic meter per day (m3/d)	m3/d, m3 d-1
	liter per second (L/s)	L/s, lps, l s-1
	mega gallon per day (MGD)	MGD
	cubic feet per minute (CFM)	CFM
Gas flow	cubic meter per second (m3/s)	m3/s, m3 s-1
	cubic meter per hour (m3/h)	m3/h, m3 h-1
	cubic meter per day (m3/d)	m3/d, m3 d-1
	liter per second (L/s)	L/s, lps, l s-1
	mega gallon per day (MGD)	MGD
	cubic feet per minute (CFM)	CFM
Gas Velocity	meter per second (m/s)	m/s
	feet per second (0.3048 m/s)	ft/s, fps, ft s-1
	inch per second (0.0254001 m/s)	in/s, ips, in s-1

#### 4.2.1.3 Asset ID

Asset ID identifies the pipe. If a network has several assets with the same name, the assets are automatically renamed to cause all pipes to have a unique Asset ID. For example two pipes named 'MyPipe' will be renamed as 'MyPipe(1)' and 'MyPipe (2)'.

#### 4.2.1.4 Node ID

Node IDs are what binds the network together and creates connectivity. Hence Node IDs must be unique. However, multiple pipes can share the same Upstream Node ID or Downstream Node ID. Therefore, Node IDs may appear in multiple cells of the network file.



#### 4.2.1.5 Link types

Mega-WATS operates with four types of links (pipes which link two nodes): gravity mains, force mains, chambers, and treatment. Other structures, such as weirs, gates, sluices, and orifices, which have a physical 'pipe length' are treated as gravity mains. The link type is given in the *link\_type* column.

All links are characterized by a length, a geometry, a material, and a pipe wall roughness. The same processes occur in all reactor types.

##### 4.2.1.5.1 Gravity pipes

Gravity pipes are the most common link type in most networks. Gravity mains are defined by the flow being driven by gravity, and the flow is calculated as semi-stationary non-uniform flow applying the Colebrook–White equation together with the Darcy friction factor. In other words, backwater is simulated but not waves. Processes are calculated assuming ideal plug flow without dispersion which is an adequate assumption as water quality changes slowly over the day.

A gravity pipe is identified by the link type (given in the *link\_type* column) containing one of the strings (case insensitive):

'grav', 'cond', 'slui', 'weir', 'gate', 'orif'.

Furthermore, if a pipe is not recognized as a force main, chamber, or treatment it will default to a gravity main. The pipe type 'Treatment' is calculated as if it were a gravity main.

##### 4.2.1.5.2 Weirs, gates, sluice and similar

Weirs, gates, sluice and similar are links but often without any upstream or downstream elevation given in the data exports from a hydrodynamic model, and they often have no diameter specified. They can be assigned a diameter (or width and height) as well as upstream and downstream elevation, just as any other link. Alternatively, one can include one column with holds information only for this type of link, giving one value for elevation (which then is assumed the same at upstream and downstream ends), and a diameter. The column identifiers for these links are *link\_diameter* and *link\_invert*, respectively. Their length is given in the *conduit\_length* column.

##### 4.2.1.5.3 Force mains

Force mains, also called rising mains or pressure mains, are calculated as always flowing full. Water transport is simply calculated based on the continuity equation. Processes are calculated assuming ideal plug flow without dispersion.

A force main is identified by the link type (given in the *link\_type* column) containing one of the strings (case insensitive):

*forc, pres, pump, pmp, rising*

##### 4.2.1.5.4 Chambers

Chambers are in-line retention tanks. Wet wells can also be simulated this way. A better approach is however to set them up as nodes (section 4.2.8). Chambers are simulated as completely mixed reactors with a headspace, a depth, and a  $K_L a$  value defined in the input file (section 4.2.1.16 and 4.2.1.17). Pipes, on the other hand, are simulated as plug flow reactors with a headspace. If no depth and  $K_L a$  values are set, the default values are used (Section 9.7).

A chamber is identified by the link type qualifier containing one of the strings (case insensitive): ‘cham’, ‘station’, ‘pit’, ‘well’.

The water depth in a chamber is controlled by the water level in the downstream gravity main. If the downstream pipe is a force main, then one must set the water level of the chamber using the “Chamber\_water\_depth” column in the network file.

#### 4.2.1.5.5 Treatment

Treatment is a special version of a gravity pipe where water phase and gas phase concentrations are set to zero, i.e., simulating a 100% effective treatment plant.

A treatment plant is identified by the link type qualifier containing the string (case insensitive) ‘treatment’.

#### 4.2.1.6 Pipe materials

Mega-WATS distinguishes between two types of pipes: Corrodible and non-corrodible ones. How fast a pipe corrodes will depend on the equivalent alkalinity set for it (section 4.2.1.13). The materials that are interpreted as corrodible are depicted in Table 4:

Table 4. Pipe materials interpreted as corrodible.

Acronym	Description
AC	Asbestos Cement
BR-CP	BRICK-CIPL Cast in Place Pipe
BR-GU	BRICK-Gunite/sprayed mortar
CO	Concrete
CONC	Concrete
CONCRETE	Concrete
IS-CP	ISP-CIPP
RC	Reinforced Concrete
RCP	Reinforced Concrete
SRCP	SRCP-Spun Reinforced Concrete Pipe
TUNNL	Concrete Reinforced Tunnel
VC-CP	VCP -CIPL
VC-RC	VCP -RCP

All names are case insensitive.

All other pipe materials are treated as non-corrodible.

If a pipe material is not given, the pipe material set in *Default network and flow settings* is assumed (Figure 38).

#### 4.2.1.7 Pipe shapes and geometry

The shapes ‘circ’, ‘rect’, and ‘trapez’ are pre-defined in WATS.

- Circular shape: The diameter of the ‘circ’ pipe is given by the ‘Diameter’ column, or if that column is not included in the network file, by the ‘Width’ column. In other words, the diameter column is not a required column, while the width and the height are. If Diameter is given, no additional values for width and height must be given in the respective columns.
- Rectangular shape: The width and height are given by the ‘Width’ and ‘Height’ columns.

- Trapezoidal shape: The trapez is basically an open channel. It has a pre-defined slope of the sides of 0.25, i.e., for each one meter of width, it rises 0.25 m. The width of the top of the trapez is given by the 'Width' column and its height by the 'Height' column. The width of the bottom is calculated based on the slope.

Other shapes are defined by a shape file, which is a text file with the name PipeShapes.prn. This file must be in the same directory as the network file.

- A new shape must start with a row containing the name of the shape: shape=MyShapeName
- Then a header row for Height and Width, separated by the Tab character (ASCII #9): Height Width
- Then comes pairs of height and width, also separated by Tab characters. Values must start from zero. A maximum number of 100 height-width pairs can be added.
- The end of a shape is defined by the word 'EndShape'.

Shapes are given as relative sizes. In other words, if a shape, e.g., an egg-shape, is defined in the shape file, the Height and Width columns will scale it. Shapes should hence range from 0 to 1 for both height and width (but don't have to, it will still work if they are not). Table 5 shows an example of a shape file with two shapes. More shapes can be added by simply adding more shapes as indicated in Table 5.

Table 5. An example of a shape file containing two shapes

shape=10.5'Marsson with FnM	
Height	Width
0	0
0.0005	0.0209
0.004	0.0626
0.0051	0.071
0.0417	0.2
0.0833	0.2764
0.125	0.3307
0.1667	0.3727
0.2083	0.4061
0.25	0.433
0.2917	0.4545
0.2986	0.4576
0.3195	0.4663
0.3333	0.4714
0.3651	0.4811
0.3933	0.9729
0.4411	0.9931
0.5	1
0.625	0.9682
0.75	0.8663
0.875	0.6614
0.9583	0.4
0.9895	0.2021
1	0
EndShape	
shape=arch	
Height	Width
0	1
0.5811	1
0.5983	0.9829
0.6838	0.9231
0.7692	0.8291
0.8547	0.6667
0.9402	0.3846
1	0
EndShape	

#### 4.2.1.8 Pipe roughness

Pipe roughness can be expressed as equivalent sand roughness as m or mm, or it can be given based on the Manning equation as Manning-M or Manning-n. Note that  $M = 1/n$  and that  $M = 25.4/(k^{1/6})$  where k is the equivalent sand roughness in m. If the roughness heading is 'eqrough' then this will always be interpreted as the equivalent sand roughness in m, irrespectively of how the selection in the setup.

#### 4.2.1.9 Pipe slope

The pipe slope is set by the user; however, Mega-WATS recalculates the pipe slope based on the upstream and downstream pipe elevation and its length. Hence this column is mainly for the convenience of the user.

#### 4.2.1.10 Upstream and downstream elevations

There are two columns related to the upstream elevation of a link. The first gives the elevation of the link invert and is identified by 'us\_invert'. The second gives the elevation of the node and is identified by 'us\_mh\_invert'. Similar for the downstream invert. Not all hydrodynamic models (from which Mega-WATS typically imports its data) operate with both, but some do. Mega-WATS only operates with upstream and downstream pipe inverts and converts this information as follows:

- If 'us\_invert' is given, the upstream link elevation is set to 'us\_invert'
- If 'us\_invert' is not given but 'us\_mh\_invert' is, the upstream link elevation is set to 'us\_mh\_invert'

#### 4.2.1.11 Coordinates of pipes

Coordinates are only used to show data on a map and Mega-WATS can as such run with wrong coordinates. Wrong or missing coordinates does of course make it difficult to work with the network.

#### 4.2.1.12 Pipe age

If available, the age of the pipes can be loaded into Mega-WATS, which then are used to predict the remaining service life (Sections 4.2.12, 7.2, and 12). A column with the qualifier 'Age' is added to the network file. The age must be given as an integer number in years, for example, 1961. If a pipe age is defined as less than 1, it is per default set equal to 1.

#### 4.2.1.13 Alkalinity of pipe material

Corrodible pipes are associated with an alkalinity. When subject to sulfuric acid formed by hydrogen sulfide oxidation (corrosion), this alkalinity is consumed. It can be set individually for each pipe in the alkalinity column (Table 2) or globally in the parameter setup menu (Section 9). The density of the material is set to 2400 kg/m<sup>3</sup>, from which the corrosion depth is calculated.

#### 4.2.1.14 Drop structures and turbulent bends

Mega-WATS identifies a drop structure from a difference in elevation between the upstream water level and downstream water level of pipes. The setup of a drop structure calculation is defined by a minimum drop height (the difference between the two water levels) and a range of parameters governing the air-water gas transfer. Turbulence and related air-water gas transfer also occurs at sharp bends, defined by a minimum angle between pipes. The parameters for gas release at drop structures and turbulent bends are set as global parameters, covering all drops in the network. Details are given in section 9.5.1.

Drop structures can be configured separately by choosing between 'fall', 'plunge', 'vortex', and 'helix' in the network setup file, column 'Drop Config'.

The drop relates always to the downstream end of the upstream pipe. A system consisting of e.g., the 3 pipes shown in Figure 13 has PupA falling into Pdw by a vortex drop and PupB falling into Pdw by a plunge drop. Hence the row for PupA must have the identifier *vortex* in its drop config column, while PupB has the

identifier *plunge*. Mass transfer effects due to the drop are assigned, respectively, to each upstream pipe's downstream node.

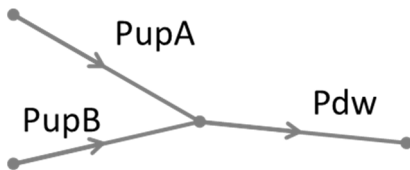


Figure 13. A simple pipe system. *PupA* falls into *Pdw* by a vortex drop and *PupB* falls into *Pdw* by a plunge drop.

#### 4.2.1.15 Overruling the default sulfide formation rate for a specific pipe

In some cases, it can be convenient to overrule the default sulfide formation rate constant used for pipes in the networks. This is done by including a column with the header *k\_sulfide*. The unit is the same as for the global default of the biofilm hydrogen sulfide formation rate constant (Section 9.4.6).

#### 4.2.1.16 Chamber water depth

The water depth in a chamber is set in a column with the header *Chamber\_water\_depth*. This overrules the default water depth set by the global parameters (Section 4.2.12).

#### 4.2.1.17 Chamber *KLa* value

The water depth in a chamber is set in a column with the header *Chamber\_KLa*. This overrules the default water depth set by the global parameters (Section 9.7).

## 4.2.2 Flow

Mega-WATS requires assignment of inflow from sub-catchments per node. From this, it calculates the hydraulics as outlined in section 4.2.1.5. The node is the structure all is hinged on, and each node hence is a unique identifier with a unique name. The nodes given in the flow file must hence correspond to the nodes in the network file. If the flow file contains nodes not included in the network file, these are simply ignored in the input. Note that Mega-WATS is case insensitive, in other words, the node MY\_NODE is the same as my\_node.

Flow files are structured as shown in: *Network, Flow and more example file.xlsx* and in Figure 14. The first row of the flow file holds the column headers which only are used to help the user know what is in each column. The text in the first row is not used for anything else.

Node ID	Total Average Flow
Units:	mgd
135-02	0.0976875
179-03	0.1119495
179-17	0.12226625
201-06	0.213045
223-24	0.0561065

Figure 14. A flow file without diurnal variation

The second row holds the units. If this row is omitted, the default values set in Mega-WATS are used (section 4.2.12, Figure 37). If some other 'unit' than the listed ones are used, Mega-WATS defaults back to the default

settings (Section 4.2.12). While loading the data, Mega-WATS shows a warning that an unknown unit was encountered.

It is recommended to include the units as a row as this ensures that Mega-WATS always interprets the units correctly.

The row holding the units must have the first column second row including the string *units* (case insensitive). The following cells then contain the unit of flow (Table 6). If it does not hold this string, the second row is interpreted as the first pipe in the network.

Table 6. Flow units permitted in the flow input data file

Description	Unit	Unit	Unit
Cubic meter per second	m3/s	m3 s-1	
Cubic meter per hour	m3/h	m3 h-1	
Cubic meter per day	m3/d	m3 d-1	
Liter per second	L/s	L s-1	lps
Mega gallon per day	mgd		
Cubic feet per minute	cfm		

The first column holds the node ID, corresponding to a node ID of the network file, where the flow value given in the second column enters the network. Note that Mega-WATS takes inflows at boundaries. Therefore, when interpreting flow input data from a hydrodynamic model, use the same input flow values as are used for the hydrodynamic model, and there is no need to export hydrographs from the hydrodynamic model.

#### 4.2.2.1 Diurnal flow variations

Using diurnal flow variations is optional. If no diurnal flow variation is to be simulated, the format of Figure 14 can be used. If diurnal flow variations are implemented, the format shown in Figure 15 must be applied, where the flow of each time step is stated in the columns following the one corresponding to the average flow.

Figure 15. A flow file with diurnal variation

Node ID	Total Average Flow	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	rr
Units:	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	mgd	rr
135-02	0.0976875	0.126598	0.115243	0.105041	0.097801	0.097812	0.103001	0.107481	0.111584	0.115764	0.114056	0.10605	0.092101	0.076134	0.064602	0.058813	0.055509	0.0
179-03	0.1119495	0.14508	0.132068	0.120377	0.112079	0.112092	0.118039	0.123173	0.127874	0.132665	0.130708	0.121533	0.105548	0.087249	0.074033	0.0674	0.063613	0.0
179-17	0.12226625	0.15845	0.144239	0.131471	0.122408	0.122422	0.128917	0.134524	0.139659	0.144891	0.142754	0.132733	0.115274	0.095289	0.080856	0.073611	0.069476	0.0
201-06	0.213045	0.276094	0.251331	0.229083	0.213292	0.213316	0.224633	0.234403	0.243351	0.252468	0.248744	0.231284	0.200862	0.166039	0.140889	0.128265	0.121059	0.1
223-24	0.0561065	0.072711	0.066189	0.06033	0.056171	0.056178	0.059158	0.061731	0.064088	0.066489	0.065508	0.06091	0.052898	0.043727	0.037104	0.033779	0.031881	0.
244-13	0.04315575	0.055927	0.050911	0.046405	0.043206	0.043211	0.045503	0.047482	0.049295	0.051141	0.050387	0.04685	0.040688	0.033634	0.028539	0.025982	0.024522	0.0

The columns following the average flow hold information regarding diurnal flow rates using the same unit as for the average flow. The number written in the header row of third column and forward is the time of the flow in hours. Hence writing -12 indicates that the time is -12 hours, then comes -11 hours, and so on. The time intervals can be freely chosen, but the shorter are the intervals, the longer will be the run time. For very large networks, one can also run out of memory if the diurnal flow variation mesh becomes too fine.

The reason to start with a negative number is based on the Mega-WATS architecture. The methodology follows the ‘buckets on a conveyor belt approach’, where water is sent downstream from upstream nodes, to then be mixed taking the travel time into account (Figure 16). Hence the calculations first become correct when all the water from all the upstream nodes have passed all the way through the network. This will typically have happened within 12 hours or less, therefore, a pre-run time of 12 hours is usually set as



default. However, the user must ascertain whether this assumption holds and, if necessary, modify the lead time (section 4.2.12, Figure 40: *Number of initial time steps ignored on graph when showing flow variation data*).

The pseudo steady state diurnal simulation approach used by Mega-WATS is highly computationally efficient. At the same time, it is fully sufficient to reproduce dry weather flow patterns even in the most complex drainage systems. It can, though, not reproduce storm water runoff events. On the other hand, sewer odor and corrosion processes are dry weather phenomena, and so there is no need to flow behavior under rain events.

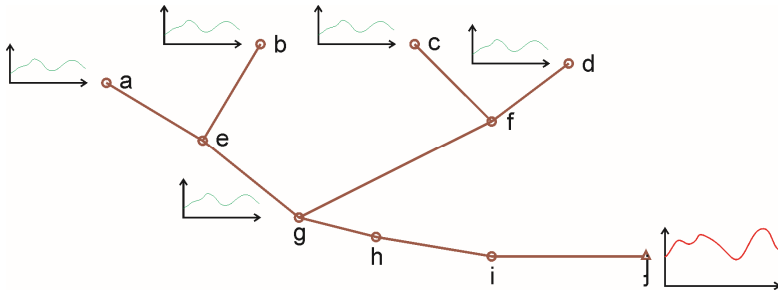


Figure 16. Mega-WATS 'buckets on a conveyor belt approach' to calculate diurnal flow variation

The flow file is loaded after the network file has been loaded (Figure 17). There are two options:

- Either not checking the 'Run flow variation' checkbox, which leads to the average flow being simulated and diurnal flow patterns ignored. In this case the average flow column is used, and the following flow columns are ignored.
- Or checking the 'Run flow variation' checkbox, which leads to the average flow column being ignored and the following flow columns being used.

After having loaded a flow file, Mega-WATS can be run (Figure 18).

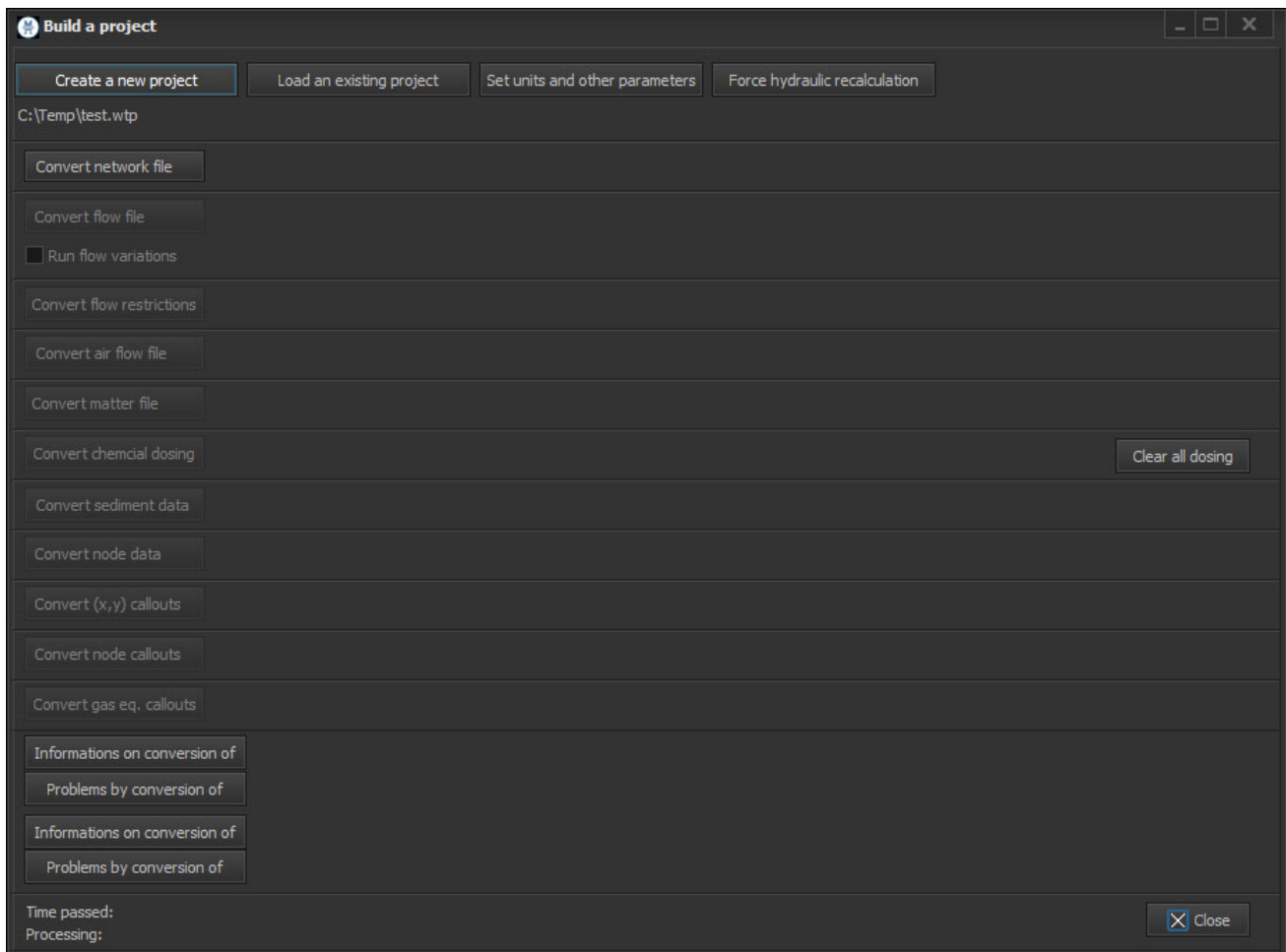


Figure 17. The project menu before creating a project

#### 4.2.3 Flow division and restriction

By far most of the nodes in a network connect one or more upstream pipes to just one downstream pipe. At some locations though, this might not be the case, and one or more upstream pipes discharge to two or more downstream pipes – a diverging fork. An example is a pumping station with two force mains. Both may be used at the same time, or maybe one is closed off while the other is in use. Or maybe one receives more water than the other. Such divergence of flow can also occur in gravity pipes. In addition, a network often holds overflows, orifices, weirs, gates, or sluices, which control or limit flow at diverging forks.

Sometimes these control structures (weirs, gates, etc.) have an elevation assigned to them, but sometimes not. If no elevation is assigned, Mega-WATS treats them as described Section 5.2, and flow is divided equally between each fork regardless of diameter and slope. If the diverging pipe(s) have elevations assigned, one link might have a lower elevation than the other. The higher pipe will then be treated as a stormwater overflow and be assumed closed during dry weather conditions. This will happen if the difference in invert levels exceeds the “Default elevation of pipe which makes it an overflow” given in the setup menu (Figure 38).

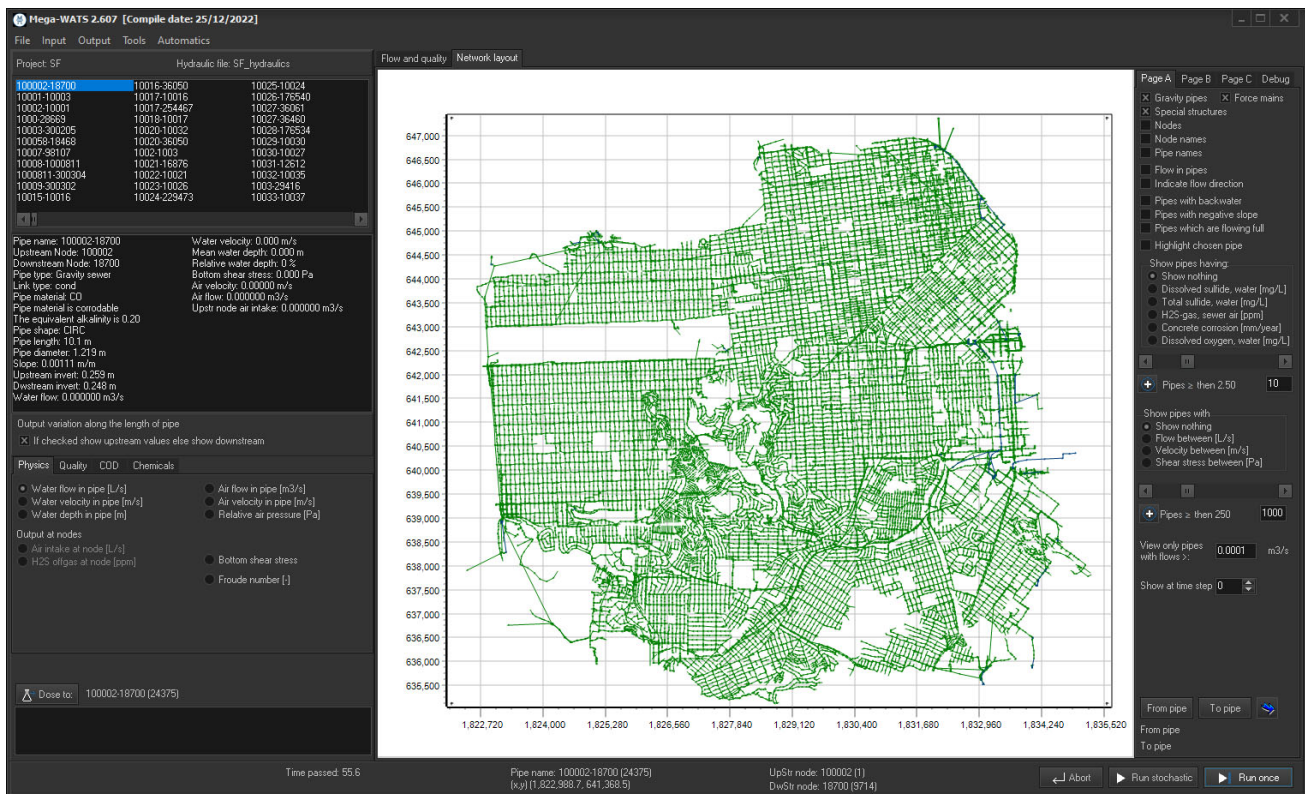


Figure 18. Mega-WATS run with a network

Where an equal flow division between forks is not correct, the user must assign the flow division in a flow restriction file. An example of how a flow restriction file is shown is in: *Network, Flow and more example file.xlsx*

The first row of the flow restriction file holds the column headers. The flow restriction file must hold the same number of diurnal flow variation time steps as the flow file (section 4.2.2). The text in the header is only to help the user getting an easier overview and the first 4 columns can contain any text. The first column holds the pipe IDs corresponding to each fork of a diverging junction. Note that in case Mega-WATS must assign new names to pipes because several pipes have the same name, it must be the new, reassigned name, which is stated in the first column.

The second column holds the operator, i.e., what is going to happen with the flow. Allowed operations are:

Divide	The fraction of the total flow that a pipe receives. The sum of the division between pipes downstream of a node must be 1. This is checked when loading a restriction file, notifying the user of errors
Restrict	The maximum flow a pipe can hold. The excess flow is spilled at the upstream end of the pipe
Restrict-Overflow	Same as just writing "restrict" but emphasizes that the excess flow is spilled (overflows) at the upstream end of the pipe
Restrict-Backwater	The maximum flow a pipe can hold. If the text also includes "backwater" then the excess flow is stemmed from the downstream end of the pipe. For the average simulation (not diurnal), a stemming period of 1 hour is assumed
Weir	The water is dammed up by a weir located at the downstream pipe invert.

The third column holds the type or unit. It can be:

Fraction	Fraction always belongs to the operator 'Divide'. When using 'Divide', one hence always must write 'Fraction' in the third column. The fraction of the upstream water sent into the pipe. The sum of fractions in the diverging pipes must equal 1. When loading a restriction file, this is automatically checked, and a list of errors is produced in case there are any. One can also subsequently click the ' <i>Check validity of flow divisions</i> ' button on the <i>Debug</i> page, which runs the same test and produces an error list.
The units of Table 6	The flow units always belong to the operator 'Restrict' or one of its sub-operators 'Restrict-Overflow' and 'Restrict-Backwater'. The flow is the maximum flow which is allowed into that pipe. If the sum of downstream flows is less than the upstream flow, water will either be spilled, or a backwater created.
m, mm, ft, in	The height units always belong to the operator 'Weir'. The value is the height of the weir crest above the pipe invert. WATS then adds the water elevation corresponding to a broad-crested weir with a weir width equal to the pipe width

If a pipe is in the flow restriction file but not in the network file, this restriction is ignored. A note of this is made in the info file which can be assessed at the form for building a project (Figure 11). If the pipe has been given an invalid operator, this is noted in the problem file. If a pipe has an invalid flow unit, the unit is set to m3/s. If a pipe has an invalid height unit, the unit is set to m.

Usually, the operation for dividing flow at a diverging fork is contained in the hydrodynamic file from which the network and flow inputs were obtained. In some cases, a flow diversion is operated at the discretion of the sewer maintenance staff, and the information must be obtained by directly questioning them.

#### 4.2.3.1 Automatic modification of flow division and restriction

Flow divisions can also be set via the graphical user interface. There are two ways to set flow divisions via the graphical user interface. Divisions can be assessed and set manually, one by one, by selecting a pipe and then pressing the button 'Change pipe flow restriction' (Figure 19).

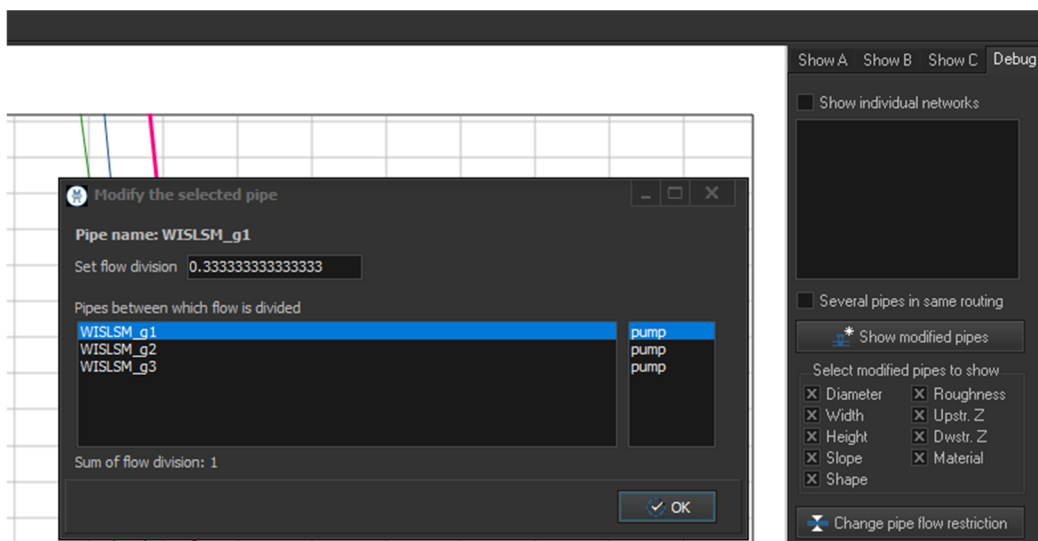


Figure 19. Change pipe flow restrictions

As discussed in the beginning of Section 4.2.3, there can though be many different pipe types in a network. For some of these one would always do the same thing, if doing it manually. For example, in case of two downstream pipes, a gravity main and a weir, most weirs would always be closed for flow in dry weather (which is the only situations simulated). In principle this should have been achieved by the elevation of the weir being higher than the gravity main, but often this information is not included in the network exports from the hydrodynamic models. Mega-WATS can therefore find and set flow divisions based on user preferences.

Click *'Auto-find flow restrictions'* on the *'Debug'* page, and up comes a menu showing all link types in the network. Chose the link type to modify. For example, as shown below, chose *'flap'* and set that it should preferably take no water. Only if it is the only way downstream for water from an upstream pipe, a flap will now allow water to flow. After having set all preferences for all pipes, press the *'auto-find flow divisions'* button.

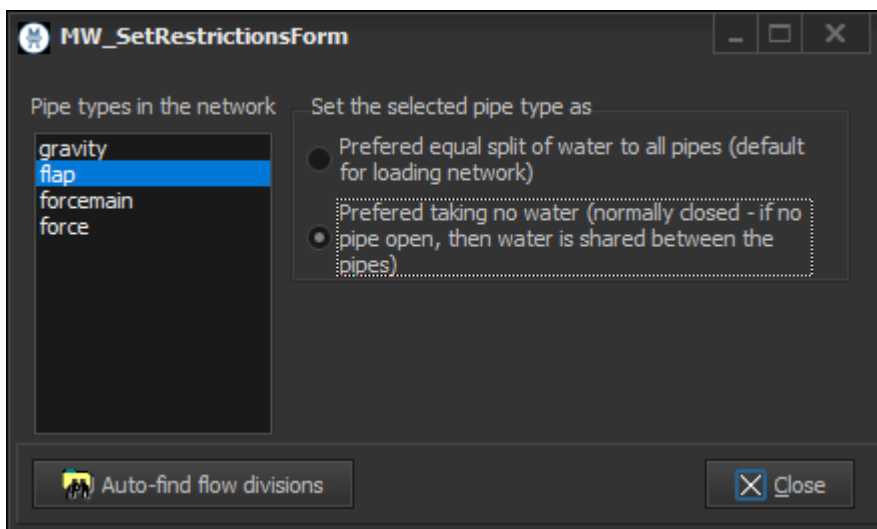


Figure 20. Menu for automatic identification of flow divisions

To test if modifications seem right, press the *'Save modifications before run'* button on the *'Debug'* page. Then run the model to see how things have taken affect.

To permanently save modifications of flow divisions, the flow restrictions must be exported using the *Tools -> Export network, flow, restrictions, chemicals* menu (Figure 21). Otherwise, the changes are lost.

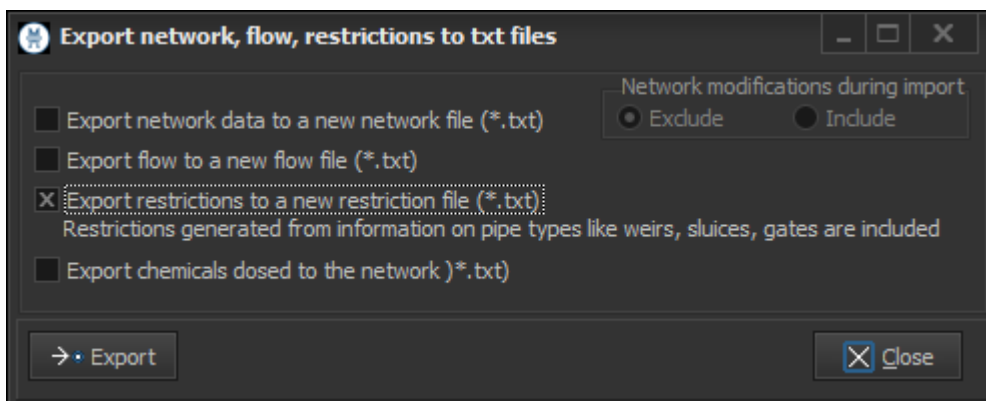


Figure 21. Export network, flow, restrictions, chemicals menu

All flow diversions can be shown by checking the 'Show flow diversions' checkbox on the 'Show B' page.

#### 4.2.4 Composition of wastewater (matter)

Water quality for every entering flow is assigned globally using the GUI menus as discussed in Section 9. Global water quality composition is appropriate for characterizing typical wastewater at in-flows, for example, fresh municipal wastewater. Certain in-flow may have different characteristics than the global values, for example flow associated with a restaurant district may have higher soluble COD, flow entering from a scalping plant may have higher volatile solids, an industry discharge may have higher pH, etc.

Global water quality values can be overruled for individual sub-catchments by using the matter file. An example of how a matter file is structured is in: *Network, Flow and more example file.xlsx*. Matter files are populated as follows:

- The first row of the matter file holds the column headers (Figure 22).
- The first column holds the node ID corresponding to the node IDs of an in-flow in the flow input file.
- The second column holds the compound for which the concentration is given, see Table 7 for admissible identifiers and units.
- The third column contains the units of the matter component.
- The fourth column holds the matter concentration for the average flow.
- The following columns hold the matter concentrations for the same time steps as the diurnal flow. The matter file must hold the same number of diurnal flow variation time steps as the flow file (Section 4.2.2).

	A	B	C	D	E	F
1	<b>Node Identifier</b>	<b>Compound</b>	<b>Units</b>	<b>Mean flow</b>	<b>-12</b>	<b>-11</b>
2	MyNode01	COD	g/m3	3500	0.2	0.2
3	MyNode02	COD	g/m3	2750	0.15	0.15

	A	B	C	D	E	F
1	<b>Node Identifier</b>	<b>Compound</b>	<b>Units</b>	<b>Mean flow</b>	<b>-12</b>	<b>-11</b>
2	MyNode01	COD	g/s	0.2	0.2	0.2
3	MyNode02	COD	g/s	0.15	0.15	0.15

Figure 22. The format of the matter file. The first version yields the concentration in g/m3, while the second version yields the matter as flux of COD to the node.



Table 7. Compounds and units for changing the chemical composition of wastewater entering a node from a sub-catchment

Identifier	Description	Units
O2	Dissolved oxygen measured as O <sub>2</sub>	g/m <sup>3</sup> , mg/L, g/L, g/s, g/h, g/d, kg/s, kg/h, kg/d
NO3	Nitrate measured as NO <sub>3</sub> -N	
NO2	Nitrite measured as NO <sub>3</sub> -N	
Fe	Total iron measured as Fe	
XFeS	Iron sulfide	
H2Sdisw	Dissolved sulfide measured as sulfide-S	
SMMw	Methyl mercaptan measured as methyl mercaptan	
SO4	Sulfate measured as SO <sub>4</sub> -S	
STracer	Tracer	
carbonate	Carbonate	mol/L, mmol/L, mol/m <sup>3</sup> , mol/s, mol/h, mol/d
amines	Amines	mol/s, mol/h, mol/d
NH3	Ammonia+ammonium	g/m <sup>3</sup> , mg/L, g/L, mol/L, mmol/L, mol/m <sup>3</sup> , mol/s, mol/h, mol/d
PO4	phosphate	mol/h, mol/d
pH	pH	-
pO2g	Partial pressure of O <sub>2</sub> in air entering the sewer	ppm, fraction
pCH3g	Partial pressure of CH <sub>4</sub> in air entering the sewer	
pCO2	Partial pressure of CO <sub>2</sub> in the sewer air	
pH2Sg	Partial pressure of H <sub>2</sub> S in the sewer air	
pMMg	Partial pressure of methyl mercaptan in the sewer air	
pTracerg	Partial pressure of tracer in sewer air	
COD can be put in either as total COD or COD fractions. If total COD is chosen, then the default distribution as given in the parameter setup is used. If both COD and its fractions is given, the last input value in the matter file will override the first. In other words, one can chose to first give total COD and then override one or more fractions individually.		
COD	Total COD measured as COD	g/m <sup>3</sup> , mg/L, g/L, g/s, g/h, g/d, kg/s, kg/h, kg/d
SF	Fermentable substrates (for example readily degradable carbohydrates)	
SA	Fermentation products (mainly VFA's)	
XHw	Heterotrophic biomass in the wastewater	
XHsulf	Sulfide forming biomass in the wastewater	
XSf	Fast hydrolysable substrates	
XSm	Medium hydrolysable substrates	
XSS	Slowly hydrolysable substrates	
XSi	Inert particulate COD	

#### 4.2.5 Dosing of chemicals and tracer substances

Several chemical treatment mechanisms are represented in Mega-WATS. These include sulfide precipitation, chemical oxidation, aerobic oxidation, anoxic oxidation, and pH adjustment. Additionally, Mega-WATS represents physical transport of a VOC tracer with user-defined properties. The chemical file is used to dose each of the chemicals shown in Table 8. Chemical management of sulfide is discussed in Section 10. Tracer analysis is discussed in Section 16.

Table 8. Compounds which can be added via the chemical addition file

Compound	Abbreviation	Conc. unit	Flux unit
Ferrous iron	Fe2	g/m3	g/s
Ferric iron	Fe3	g/m3	g/s
Nitrate (measured as NO3-N)	NO3	g/m3	g/s
Oxygen	O2	g/m3	g/s
Hydrogen peroxide (measured as H2O2 mass)	H2O2	g/m3	g/s
Hypochlorite (measured as OCl mass)	OCl	g/m3	g/s
Base (measured in moles)	Base	mol/m3	mol/s
Magnesium hydroxide (measured in Mg mass)	Mg(OH)2	g/m3	g/s
Tracer in the water	TracerW	g/m3	g/s
Tracer in the air	TracerG	g/m3	g/s

An example of how a dosing file is structured is in: *Network, Flow and more example file.xlsx* which is an addendum to this manual. The chemical file is populated as follows:

- The first row of the dosing file holds the column headers. The dosing file must hold the same number of diurnal flow variation time steps as the flow file (Section 4.2.2). Which text to choose for the first four columns of the first row is up to the user and does not affect the simulations.
- The first column holds the pipe ID, corresponding to the pipe IDs of the network file. Dosing occurs at the upstream end of that pipe.
- The second column holds the chemical to dose. Admissible identifiers are presented in Table 8.
- The third column holds the dosing pattern and unit. The dosing pattern can either be flow proportional, in which case the unit is g/m<sup>3</sup> for all substances but the base, for which it is mol/m<sup>3</sup> (or mole/m<sup>3</sup>). Or it can be time proportional, in which case the unit is g/s for all substances but the base, for which it is mol/s (or mole/s).
- The fourth column holds the average dose using the unit defined in the third column.

Pipe (dosing at upstream node)	Component	Dosing pattern	Mean flow
23869a-23869b	Fe2	g/m3	5
86166-10662	Fe2	g/s	2.46
109419-101841	Fe2	g/s	4.92

Figure 23. A chemical dosing file without diurnal variation

The following columns hold information regarding diurnal dosing rates. The number written in the header row of the fifth column and forward is the time of the flow, like for the water flow time steps (section 4.2.2).

#### 4.2.6 Sewer air flow files

Mega-WATS calculates the air flow in the sewers based on a momentum balance between the water dragging the air and the pipe wall above the waterline restricting the flow. When the air flow in an upstream pipe is larger than in a downstream pipe, air is released from the connecting node. If the air flow in an

upstream pipe is smaller than a downstream pipe, air is taken in at the connecting node. This results in the air always flowing in the same direction as the water. This default treatment of headspace air flow errs toward an assumption of ‘openness’ to the atmosphere at every node. These provisional air flow values can be overruled by a gas flow file. In this file, the actual air flow or air velocity is given for each pipe and used instead of the provisional values calculated by Mega-WATS. Usually, the sewer headspace is sealed to some extent with openings to atmosphere constrained by vents or pick holes. Representation of ‘sealedness’ and resulting pressurization, the influence of fans, and counter-current air flow can be accomplished by completing a Mega-Vent model which treats headspace air pressure/flow specifically. The Mega-Vent results can then be over-laid into Mega-WATS using the air flow file.

An example of how a gas flow file is structured is provided in: *Network, Flow and more example file.xlsx* and shown in Figure 24.

The first row of the air flow file holds the column headers. The air flow file must hold the same number of diurnal flow variation time steps as the flow file (section 4.2.2).

Asset ID	Air flow	Upstr node pressure	Downstr node pressure
Units:	m3/s	Pa	Pa
78409148	0	101325	101325
78528988	0	101325	101325

Figure 24. Air flow file without diurnal variation

The first column holds the pipe ID, corresponding to the pipe IDs of the network file. The second column holds the unit of the flow. Admissible units are given in Table 9. The third and fourth columns hold the upstream and downstream air pressures.

Table 9. Admissible units for the gas flow file

Unit	Type	Explanation
m/s	Gas velocity	meter per second
fps	Gas velocity	feet per second
m3/s	Gas flow rate	cubic meter per second
m3/h	Gas flow rate	cubic meter per hour
L/s	Gas flow rate	Liter per second
CFH	Gas flow rate	cubic feet per hour
CFM	Gas flow rate	cubic feet per minute
CFS	Gas flow rate	cubic feet per second

For diurnal flow, the air flow rate, and upstream and downstream pressures are continued for each time step (Figure 25).

Asset ID	Air flow	Upstr node pressure	Downstr node pressure	-12	-11	-10
Units:	m3/s	Pa	Pa	m3/s	Pa	Pa
78409148	0	101325	101325	0	101325	101325
78528988	0	101325	101325	0	101325	101325

Figure 25. Air flow file with diurnal variation

#### 4.2.7 Sediment data

A pipe can be assigned a sediment layer in case such has been measured or deduced by another approach such as shear analysis. A layer of sediment changes the profile of a pipe, for example, if a circular pipe is partly filled by sediments, it is no longer circular (Figure 26). Mega-WATS calculates the hydraulics based on the new shape created by the sediments in the pipe. The sediments furthermore affect sulfide formation by some factor, which can be set in *Simulation parameters*, page *Sulfide form. biofilm*, lower grid, first and second row (Section 9.4.6).



Figure 26. A pipe with and without sediments

An example of how a sediment depth file is structured is in: *Network, Flow and more example file.xlsx*

The format of the sediment file consists of a header row, a units row, and rows with pipe names and associated sediment depths (Figure 27).

Asset ID	Sediment depth
Units:	mm
BM46_BM45	30
BM47_BM46	40
BM48_BM47	35
BM49_BM48	50
BM50_BM49	55

m	meter	metre
cm	centimeter	centimetre
mm	millimeter	millimetre
in	inch	inches
ft	feet	foot

Figure 27. The sediment file format (left) and the allowed units for the sediment depth

The sediment data can be shown by checking the *Pipe sediments* > checkbox on the *Show B* page. The sediments are also visible when drawing a pipe profile (Figure 28).

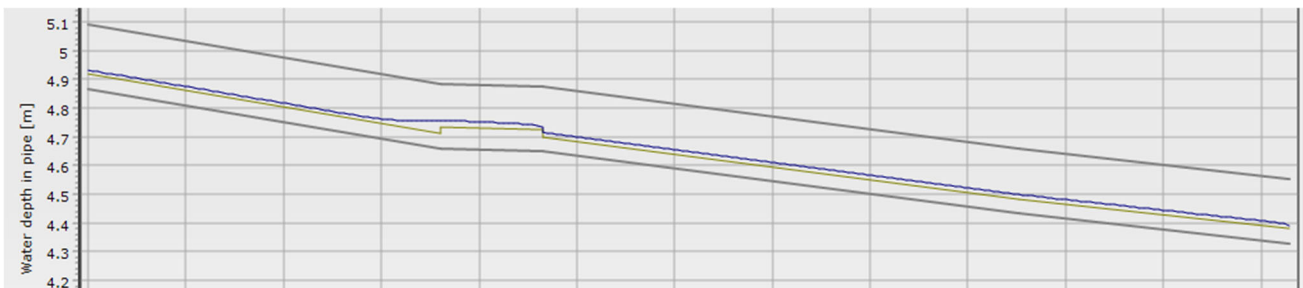


Figure 28. Example of a stretch of pipes with sediments

#### 4.2.8 Nodes as Well-Mixed Reactors

Nodes are as default assumed to have no volume, neither for water nor air. This can be overridden by loading node data where a node is assigned a volume in which processes can proceed, for example wet wells. Another example is a manhole to simulate its corrosion. The input format for nodes is shown in Figure 29 and Figure 30 for simulation of average conditions.

- The first column holds the node IDs (section 4.2.1)
- The second column holds the invert elevation, i.e., the bottom of the node. Make sure the invert is equal to or lower than then the downstream invert of all pipes leading to the node.
- Then comes the water level in the node. Make sure it is above the invert.
- The roof level (top of the node) must be higher than the water level
- The shape can be circular (*circ*) or rectangular (*rect*, *cube*, *square* all work as identifier)
- Width is the width if rectangular or the diameter if circular
- Length is the length if rectangular
- Materials are the same as pipe materials (section 4.2.1.6)
- Node KLa is the reaeration rate of the water in the node
- Gooseneck vent diameter is optional. It adds a gooseneck pipe to the node with the purpose of adding air to the node
- Gooseneck vent flow is optional. It sets the amount of air flow to the gooseneck. Both the diameter and the gas flow must be added to make goosenecks work

Node ID	Invert level	Water level	Roof level	Shape	Width	Length	Material	Node KLa	GooseNeck Diameter	Gooseneck gas flow rate
Units:	m	m	m		m	m		1/d	m	m <sup>3</sup> /s
SAXSSP	0.1	1.1	2.4	rect	2	2	conc	20	100	0.001
SAXHSM	0.2	1.2	2.5	rect	2	2	conc	20	100	0.001

Figure 29. Input format for node data with gooseneck and without diurnal flow variation

Node ID	Invert level	Water level	Roof level	Shape	Width	Length	Material	Node KLa
Units:	m	m	m		m	m		1/d
SAXSSP	0.1	1.1	2.4	rect	2	2	conc	20
SAXHSM	0.2	1.2	2.5	rect	2	2	conc	20

Figure 30. Input format for node data without gooseneck and without diurnal flow variation

See also the “*Network, flow and more example file*”.

If the purpose solely is to simulate manhole corrosion, the water level of the node should be set to the invert level. This suppresses simulation of processes in a ‘water volume’ in the node. Gooseneck diameter and air flow rate should be set to zero.

##### 4.2.8.1 Visualizing node information

The node information can be shown in detail by checking the Nodes checkbox on Page A of the main form (Figure 1) and double-clicking on the node of interest. A form with information is then shown (Figure 31).

It is also possible to only show the loaded nodes pressing one of the buttons (*Page B*) *Loaded nodes with water* or *All loaded nodes*. This shows only the loaded nodes, which might be more convenient.

301016		No. 26021		301016		No. 26021		301016		No. 26021	
Node total volume [m <sup>3</sup> ]	7964.113	H2S gas [ppm]	0.00	Dis. sulfide [mg/L]	0.02						
Node water volume [m <sup>3</sup> ]	2867.081	Methyl Merc. gas [ppm]	0.003	Methyl Merc. [mg/L]	0.000						
Node air volume [m <sup>3</sup> ]	5097.032	CO2 gas [ppm]	771.1	Total COD [mg/L]	632.7						
Water intake [m <sup>3</sup> /s]	0.000000	O2 gas [ppm]	205133	Dis. oxygen [mg/L]	0.09						
Air intake [m <sup>3</sup> /s]	-17.266515	Methane gas [ppm]	0.00	Dis. methane [mg/L]	0.000						
Water residence time [h]	1.107661	Tracer gas [ppm]	0.00	Dis. tracer [ppm]	0.00						
Gooseneck Qair [m <sup>3</sup> ]	1.000	Conc. corrosion [mm/y]	0.01	pH [-]	8.40						

Pipes entering node	Qwater	Qgas	pH2S	pMM	pCH4	pCO2	pO2	Dis. sulfide	Methyl merc	Dis. methan	Dis. oxygen	pH	Conc. corr.
	[m <sup>3</sup> /s]	[m <sup>3</sup> /s]	[ppm]	[ppm]	[ppm]	[ppm]	[ppm]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[-]	[mm/y]
301014-301016	0.719003	16.266515	0.02	0.001	0.00	997.6	209471	0.07	0.000	0.000	7.70	8.59	0.04
GooseNeck301016	0.000000	1.000000	0.00	0.000	0.00	1000.0	209500	0.00	0.000	0.000	0.00	0.00	0.00

Pipes exiting node	Qwater	Qgas	pH2S	pMM	pCH4	pCO2	pO2	Dis. sulfide	Methyl merc	Dis. methan	Dis. oxygen	pH	Conc. corr.
	[m <sup>3</sup> /s]	[m <sup>3</sup> /s]	[ppm]	[ppm]	[ppm]	[ppm]	[ppm]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[-]	[mm/y]
301016-301018(1)	0.359501	0.000000	0.00	0.003	0.00	771.1	205133	0.02	0.000	0.000	0.09	8.40	0.00
301016-301018(2)	0.359501	0.000000	0.00	0.003	0.00	771.1	205133	0.02	0.000	0.000	0.09	8.40	0.00

Figure 31. Information on nodes after double-clicking a node to which a volume and etcetera has been assigned

On the main form, further info can be displayed by a flow path going through the node of interest. The water depth through the node presented in Figure 31 is shown in Figure 32. Various water quality parameters in the node are also shown on the flow path graphs, for example the dissolved sulfide in Figure 33. In this example, sulfide was formed in the wet well due to a water residence time of 3 hours and the reaeration set quite low ( $K_L a = 20 \text{ d}^{-1}$ ). Choosing different parameters, e.g., a smaller wet well and higher reaeration would of course have change this.



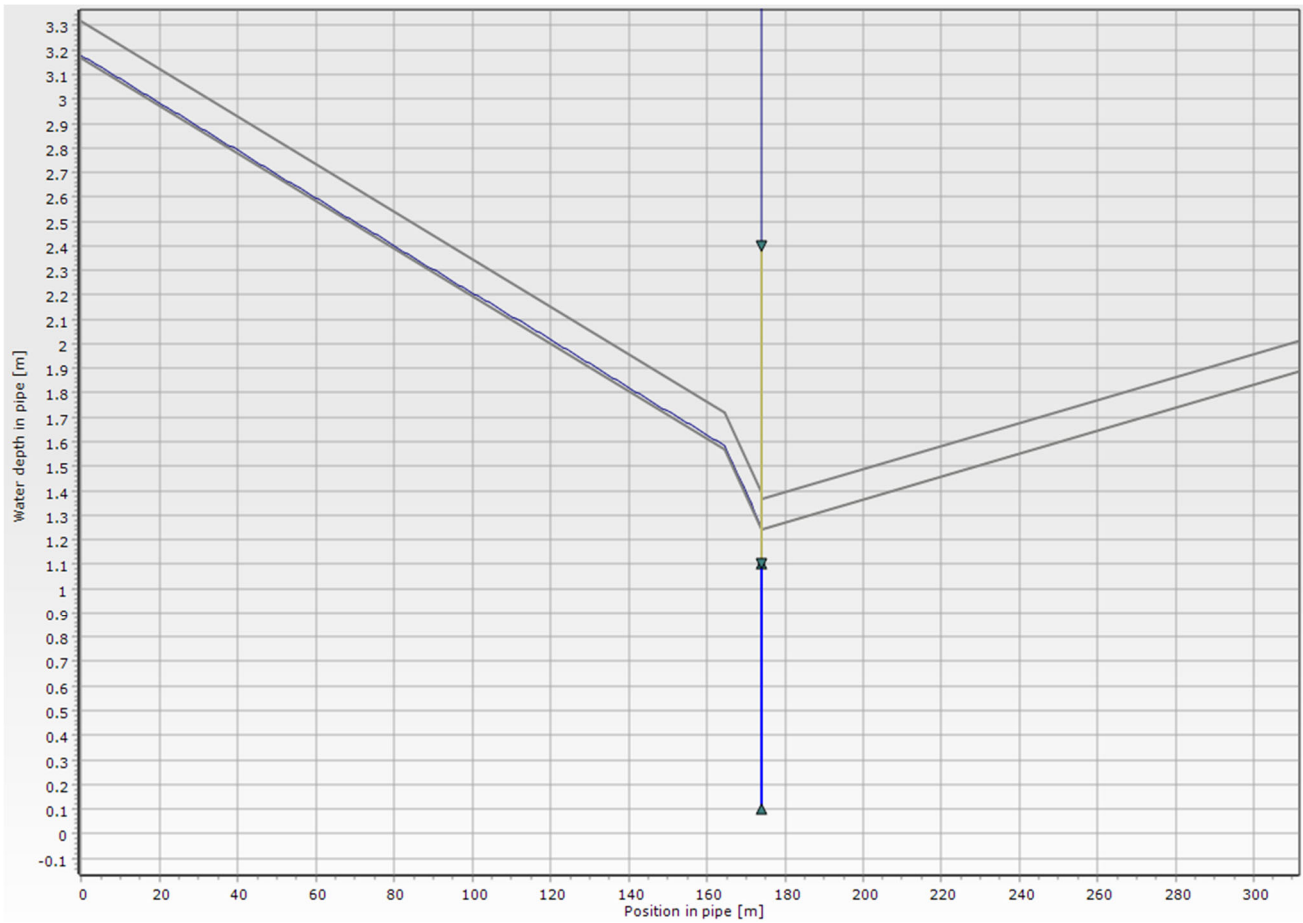


Figure 32. Flow path through the node presented in Figure 31. The vertical blue line indicates the water in the pond, starting at the lower triangle at the pipe invert ending at the two triangles point towards each other. The yellow line indicates the air in the node, ending in a triangle pointing downwards. The vertical line above the air is the pressure level in the force main and hence not related to the node.

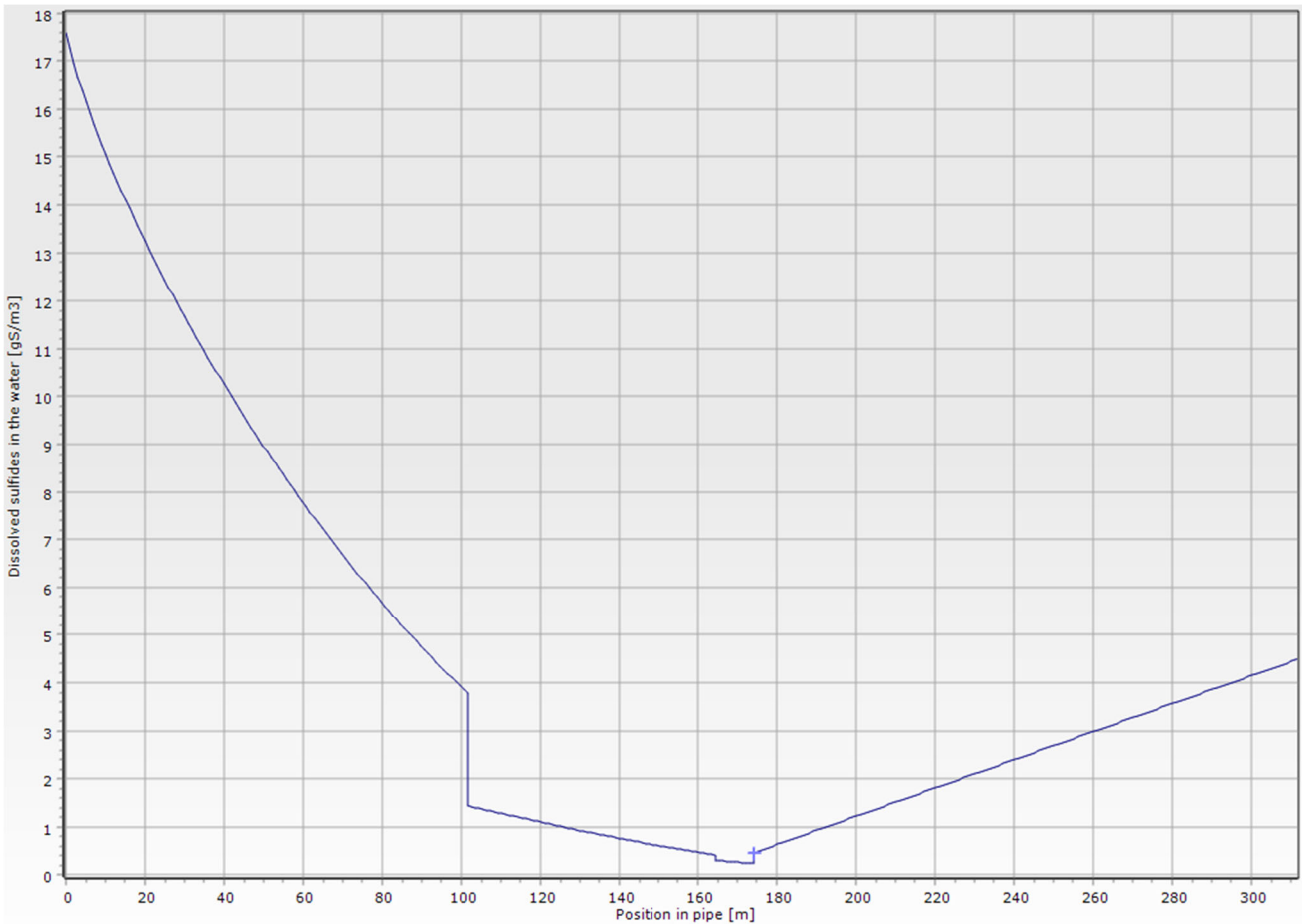


Figure 33. Flow path through the node presented in Figure 31. The blue cross at position 175 m indicates the dissolve sulfide concentration in the wet well

#### 4.2.8.2 Diurnal node variations

Nodes can have diurnal variation of water level, node  $K_La$ , and gooseneck gas flow rate. This is achieved by adding columns for water level, node  $K_La$ , and gooseneck gas flow rate for each time step (Figure 34). If Goosenecks are omitted, then only add columns for water level and node  $K_La$  (Figure 35).

Node ID	Invert level	Water level	Roof level	Shape	Width	Length	Material	Node $K_La$	GooseNeck Diameter	GooseNeck gas flow rate	-12	-11	-10	-9	-8													
Units:	m	m	m		m	m		1/d	m	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s
SAXSSP	0.1	1.1	2.4	rect	2	2	conc	20	100	0.001	1.1	22	0.0011	1.2	24	0.0012	1.3	26	0.0013	1.3	26	0.0013	1.2	24	0.0012	1.3	26	0.0013
SAXHSM	0.2	1.2	2.5	rect	2	2	conc	20	100	0.001	1.2	24	0.0012	1.3	26	0.0013	1.5	30	0.0015	1.5	30	0.0015	1.3	26	0.0013	1.5	30	0.0015

-12	-11	-10	-9	-8										
m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s	m	1/d	m³/s
1.1	22	0.0011	1.2	24	0.0012	1.3	26	0.0013	1.3	26	0.0013	1.2	24	0.0012
1.2	24	0.0012	1.3	26	0.0013	1.5	30	0.0015	1.5	30	0.0015	1.3	26	0.0013

Figure 34. Input format for node data with gooseneck and with diurnal flow variation

Node ID	Invert level	Water level	Roof level	Shape	Width	Length	Material	Node KLa	-12	-11	-10	-9	-8	-7	-6	-5
Units:	m	m	m		m	m		1/d	m	1/d	m	1/d	m	1/d	m	1/d
SAXSSP	0.1	1.1	2.4	rect	2		2 conc	20	1.1	22	1.2	24	1.3	26	1.3	26
SAXHSM	0.2	1.2	2.5	rect	2		2 conc	20	1.2	24	1.3	26	1.5	30	1.5	30

-12	-11	-10	-9	-8	-7	-6	-5
m	1/d	m	1/d	m	1/d	m	1/d
1.1	22	1.2	24	1.3	26	1.3	26
1.2	24	1.3	26	1.5	30	1.5	30

Figure 35. Input format for node data without gooseneck and with diurnal flow variation

#### 4.2.9 Callouts at [x,y] coordinates

Callouts can be shown at specified x,y-coordinates by loading a text file of the format:

x (longitude)	y (latitude)	Label	RGB red	RGB green	RGB blue
489691	375349	Odor complaint	204	255	150
490103	374997	Odor complaint	204	255	150
489321	375624	Odor complaint	204	255	150

An example of how a callout file is structured is in: *Network, Flow and more example file.xlsx*

The x (longitude) and y (latitude) refer to the coordinates on the map and must be in the same system and unit as the coordinates of pipes and nodes in the network file. The label contains text which can be displayed at the callouts. The RGB colors refer to the color coding of the RGB system, where each color tone is represented by a byte-value, i.e., the three tones (red, green, blue) have values between 0 and 255. For example, is (255, 0, 0) a strong red, (0, 255, 0) a strong green, and (0, 0, 255) a strong blue. For more info on RGB colors see [https://www.rapidtables.com/web/color/RGB\\_Color.html](https://www.rapidtables.com/web/color/RGB_Color.html) or similar webpages.

The label can be shown or hidden by checking *Show the label of the (x,y) callout* checkbox on the *Show B* page.

The size of the callout marker can be changed in the setup menu: *Tools* → *Default network and flow settings* → the tab *Graph scaling*.

#### 4.2.10 Callouts at nodes

Callouts can be shown at specified nodes by loading a text file of the format:

Node ID	Label	RGB red	RGB green	RGB blue
V0116	C1	204	255	150
TF46140198	C2	204	255	150
MC_WALNUT_SCREW	C3	204	255	150
125555A	C4	204	255	150

An example of how a callout file is structured is in: *Network, Flow and more example file.xlsx*

Node ID refers to a node in the network file. The label contains text which can be displayed at the callouts. The RGB colors refer to the color coding of the RGB system, where each color tone is represented by a byte-value, i.e., the three tones (red, green, blue) have values between 0 and 255. For example, is (255, 0, 0) a

strong red, (0, 255, 0) a strong green, and (0, 0, 255) a strong blue. For more info on RGB colors see [https://www.rapidtables.com/web/color/RGB\\_Color.html](https://www.rapidtables.com/web/color/RGB_Color.html) or similar webpages.

The label can be shown or hidden by checking the *Show the label of the node callout* checkbox on the *Show B* page.

The size of the callout marker can be changed in the setup menu: *Tools* → *Default network and flow settings* → the tab *Graph scaling*.

#### 4.2.11 Gas equilibrium callouts at nodes

Mega-WATS can show the water-gas equilibrium concentration for gases at nodes even though there is no air phase at the node. This is for example relevant when assessing what the concentration of off-gases from air release valves, or at pipes where air flow is zero for other reasons. Gases that can be shown are H<sub>2</sub>S and MM (methanethiol, also known as methyl mercaptan).

A text file containing the node ID and what to show is loaded into the *Build a project* form (Figure 11). The file format is:

Node ID	Node type	RGB red	RGB green	RGB blue
V0424	H2S equilibrium	204	255	150
V0414	MM equilibrium	100	255	100
TF46116201	H2S equilibrium	204	255	150
TF47103805	MM equilibrium	100	255	100

An example of how a callout file is structured is in: *Network, Flow and more example file.xlsx*

Node ID refers to a node in the network file. The label contains text which can be displayed at the callouts. The node type identifier H<sub>2</sub>S will cause gas-water equilibrium concentrations H<sub>2</sub>S gas to be shown while MM will cause methanethiol (methyl mercaptan) to be shown.

The RGB colors refer to the color coding of the RGB system, where each color tone is represented by a byte-value, i.e., the three tones (red, green, blue) have values between 0 and 255. For example, is (255, 0, 0) a strong red, (0, 255, 0) a strong green, and (0, 0, 255) a strong blue. For more info on RGB colors see for [https://www.rapidtables.com/web/color/RGB\\_Color.html](https://www.rapidtables.com/web/color/RGB_Color.html) or similar webpages.

These data can be loaded either before or after a simulation is run.

To view the output data, go to the page *Show B* and press the *Gas equilibrium at nodes* button. An example of the output is shown in Figure 36. This option to show data only makes sense when running average concentrations, as only one value is shown per node.

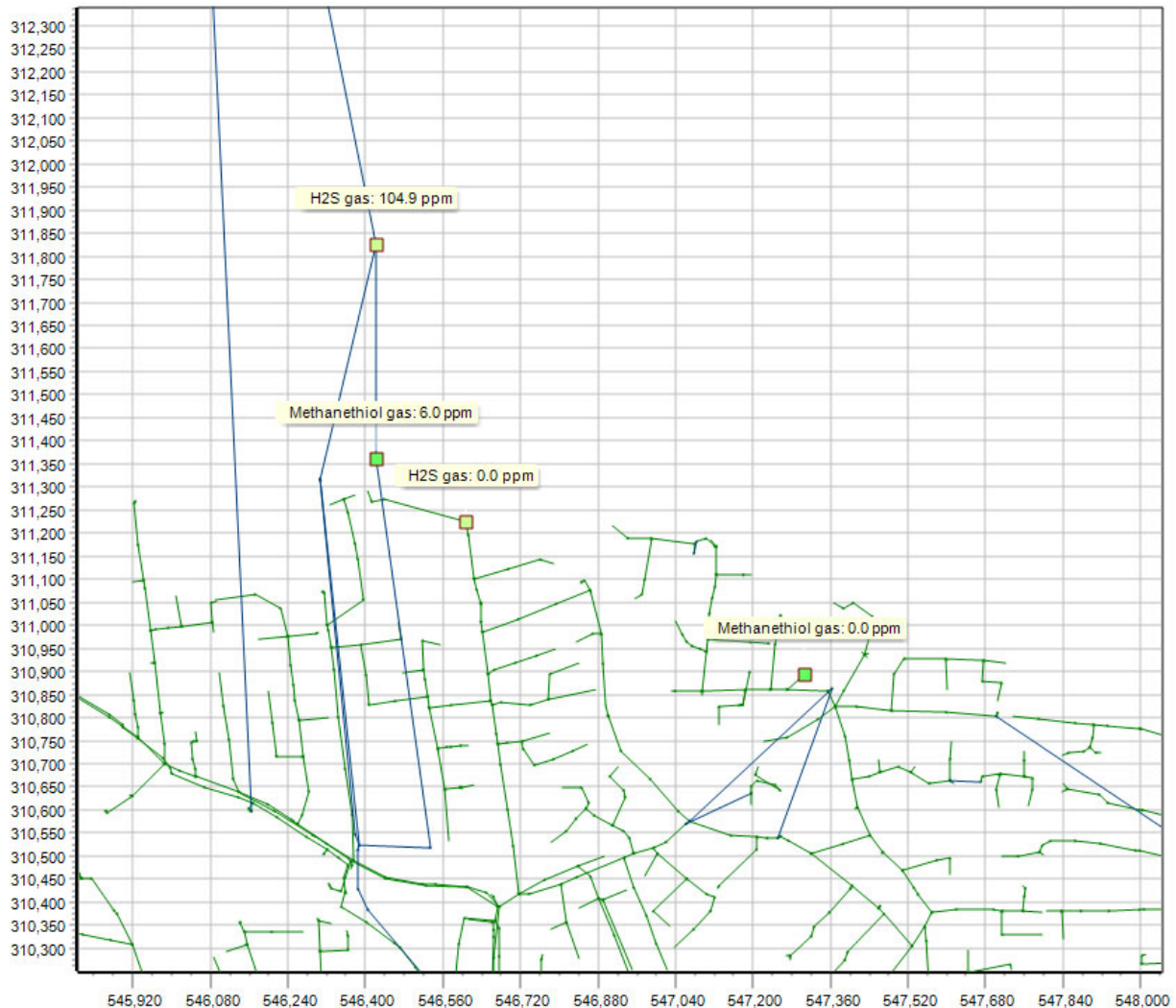


Figure 36. An example of equilibrium concentrations at nodes

#### 4.2.12 Default GUI Graphics Scale, Network Settings, and Flow Settings

The default settings can be accessed via *Tools* → *Default network and flow settings* → the tab *Graph scaling* or via *Input* → *Load or build a project file* → the button *Set units and other parameters*.

In the lower left corner of the form, there is a button called *Reset to factory defaults*, which is visible for all pages of the form. It sets all Mega-WATS parameters to their default settings. This form holds pages with various setups:

The page *Units of datafiles* (Figure 37) sets the default units of network and flow files, which are used in case no unit row is given in the datafiles (which is not recommended), or in case the unit cannot be recognized (e.g. due to a spelling error like writing n3/s instead of m3/s). There are four buttons for default units which can be of help to set such rapidly.

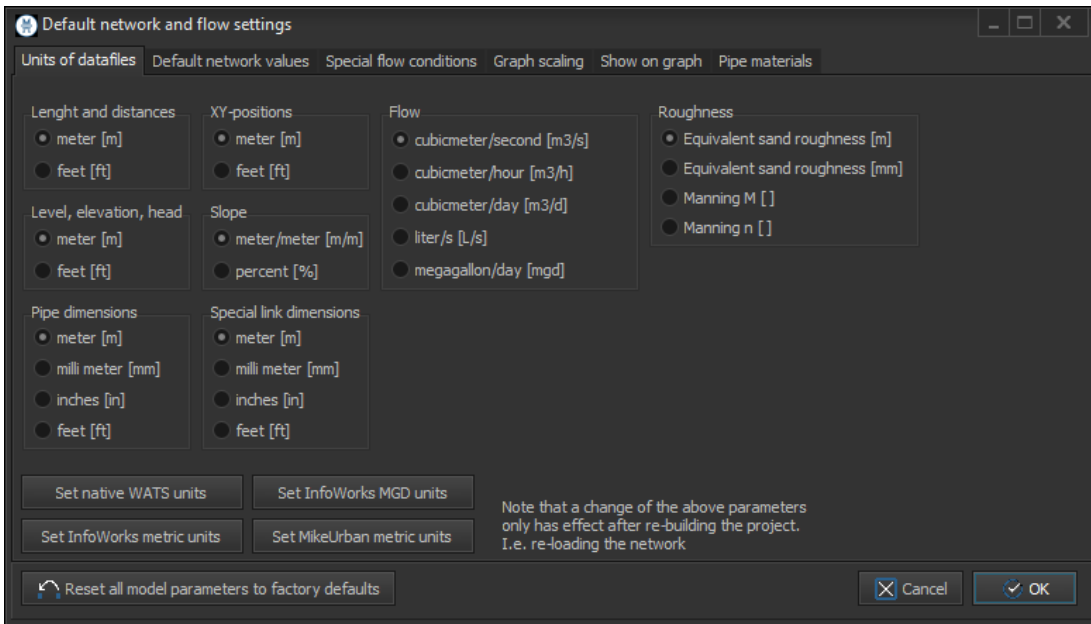


Figure 37. Default unit settings

The *Default network values* page holds some default values which are used when information is missing or out of reasonable bounds (Figure 38).



Figure 38. Default network values

The *Special flow conditions* page (Figure 39) sets restriction on the flow velocity in a full-flowing pipe. These values act as restrictions to the flow, simply because it is unrealistic that water can flow that fast in a pipe. Water exceeding those capacities will be spilled. The rationale behind this parameter is that such flows most likely are caused by some sort of error in the data file.

It also sets the simulated time before breaking out of the calculation of a single pipe (typically a force main). If flow in a force main is extremely slow, the model could crunch on that pipe for a long time. Most likely



such long residence time is an error in the data. Pipes which are very slow to calculate can found from the *Debug page, Information on network* and then *Show slow pipes* (Section 5.3.5).

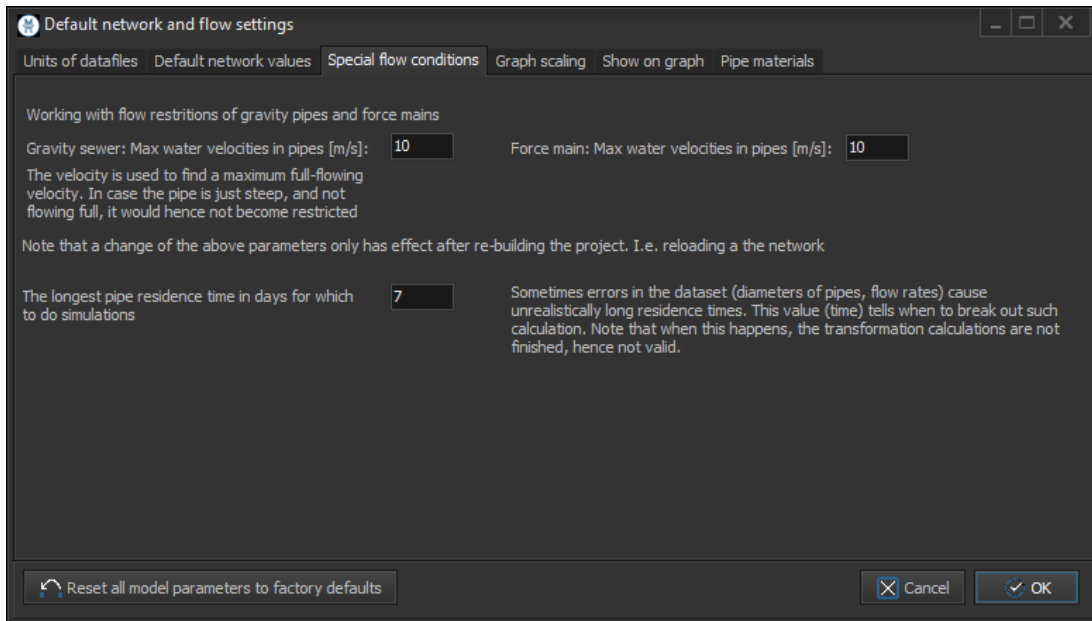


Figure 39. Values for special flow conditions

The *Graph scaling* page (Figure 40) sets various parameters related to the graphics.

In the top left corner is a checkbox called *Force fixed scale on graphs*. Checking it and at the same time filling in the scale range in the edit fields *Fixed max y-scale of graph* and *Fixed min y-scale of graph* locks all graphics to a fixed scale. This is useful when copying graphs directly from Mega-WATS for presentation purposes.

The font of the axis labels and title can be set using the *Axis label font size* and *Axis title font size* spin buttons.

The font of the text when showing node names, pipe names, and flows on the map (*Page A*) can be set by *Node names*, *Pipe names*, and *Flow* spin edit boxes.

The font and decimals of outgas marks (*Page C*) can be set using the *Outgas marks* spin buttons.

The *Number of initial time steps ignored on graph when showing flow variation data* sets how many time steps are ignored when showing diurnal simulations (section 4.2.2.1).

The sizes of callout markers and hydraulic jump markers as well as their shape are set by *Size of ... marker*.

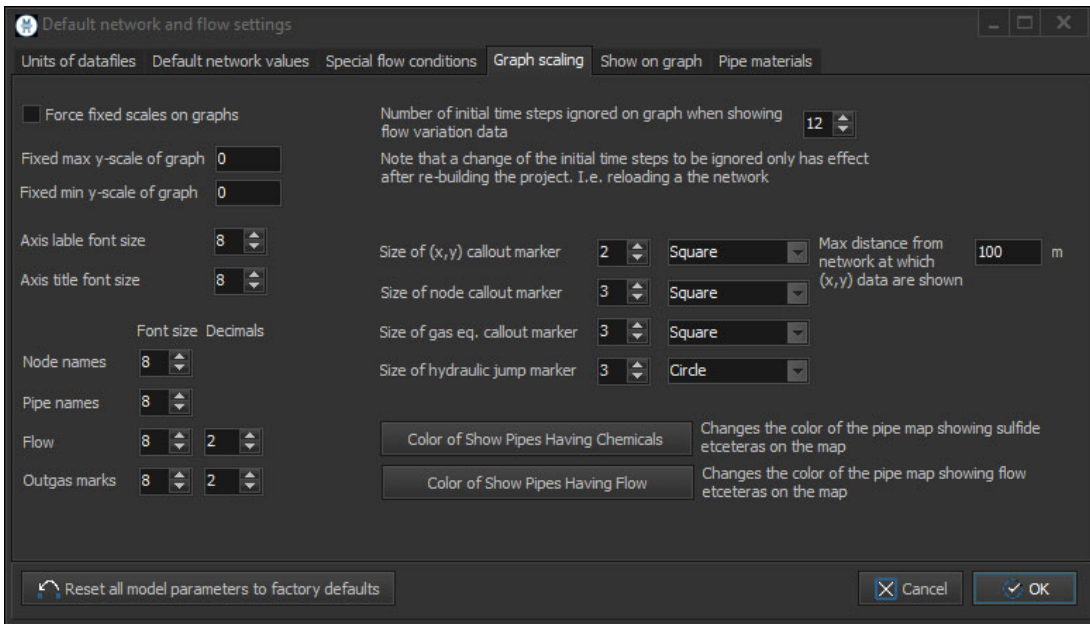


Figure 40. Values for graph scaling and more

The *Show on graph* page (Figure 41) allows the user to view data from diurnal simulations in two ways. Either as diurnal profiles where the profiles are shown for upstream and downstream ends of each pipe, or for a selected time step where the full pipe length of the pipes can be used, for example using flow path's (Section 5.6).

This page also holds the setting for when to show pipes with backwater when choosing *Pipes with backwater* on Page A.

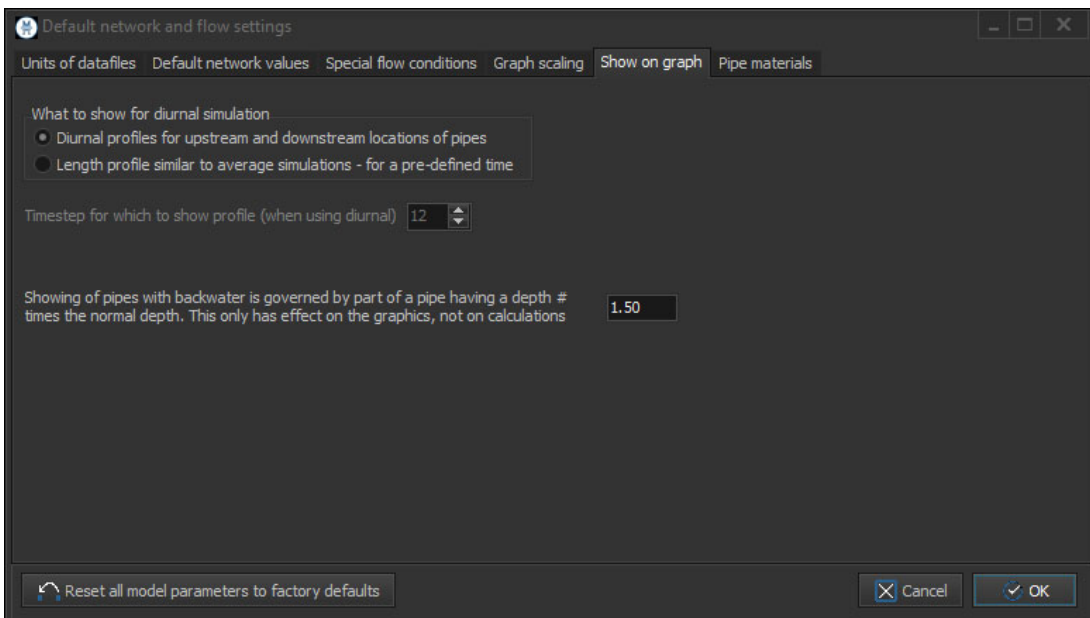


Figure 41. What to show on graphs for diurnal simulations. Relative value above which backwater is shown

The page *Pipe materials* shows all the pipe materials in the loaded network, and indicates which are corrodible (Figure 42). To the right of the pipe materials, there are settings for predicting remaining life of the pipes. For this to work, the pipe age should be loaded in the network file (Section 4.2.1.12). The *Factor*

times diameter yielding pipe wall loss to failure and the Maximum pipe wall loss before failure [mm] are used to automatically generate the Loss to failure table on the right hand of the form. The Loss to failure table entries can be manually modified.

The Factor to account for the simulated corrosion being the average along the moist pipe perimeter considers that corrosion is not homogeneously distributed along the pipe wall.

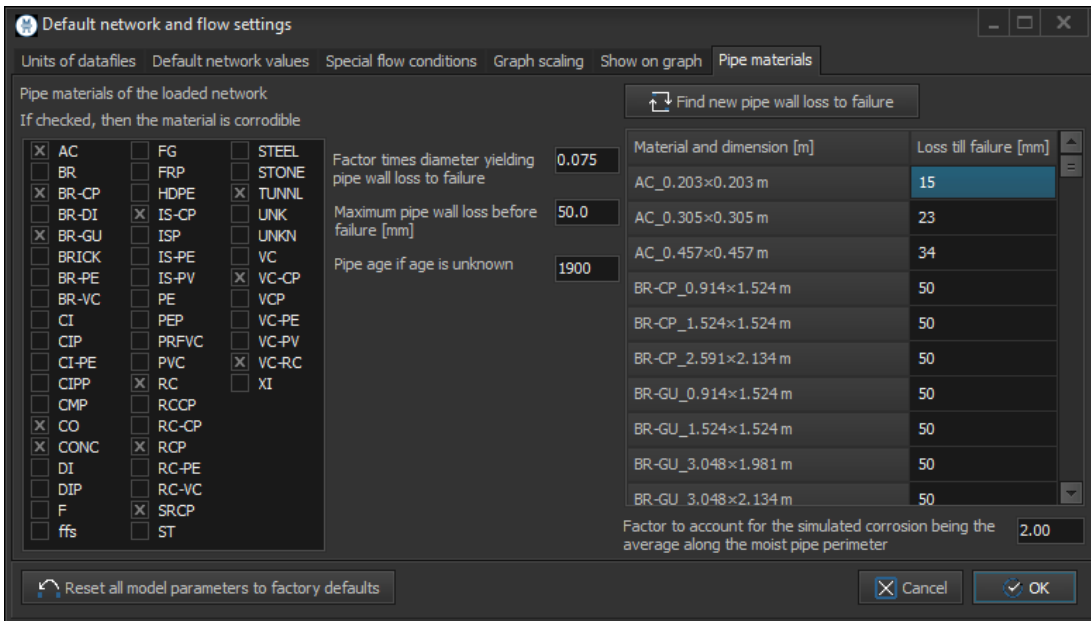


Figure 42. Pipe materials in the network and whether these are corrodible or not, as well as the allowed corrosion before end of service life (section 7.2)

See also Section 7.2.

## 5 Debugging and modifying networks, getting information

It is quite common that there are many errors and missing information in a network file when one extracts it from, for example, a hydrodynamic model. These must be identified and debugged before the model can be trusted. Mega-WATS therefore has several tools which help setting up networks and identify common problems in the setup of networks.

### 5.1 Export network, flow, restrictions to txt files

The network file, a flow file, and the restriction file used to generate the WATS data files are TAB separated txt files (section 4.2.1). One can export the Mega-WATS data files back to the original TAB separated txt file format.

*Tools → Export modified network and restrictions*

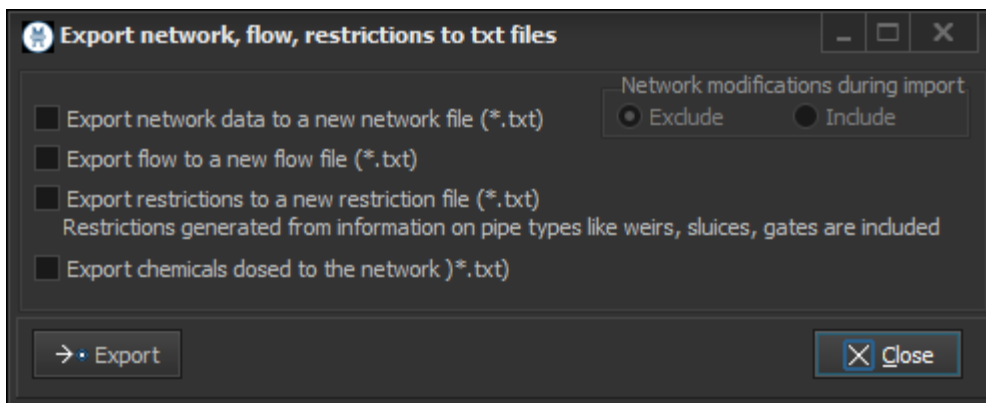


Figure 43. Exporting Mega-WATS network data back to text files

**Export network data:** When Mega-WATS builds the network file, it automatically generates some modifications from the network txt file when there are encountered inconsistencies or when some parameters, e.g., pipe roughness, are out of the predefined boundaries. The modified network file can be exported back to a TAB separated txt file. This can be done with or without info on what was modified. Click the 'Export network data to a new network file (\*.txt)'. The option to exclude or include information on what was modified now becomes active. The default is *exclude*. Press *Export* to export the data. If one chose to include info on modifications, the resulting files ads columns telling which pipes and parameters were modified (writing 'true' in the relevant cell).

**Export flow data:** When WATS builds the flow file, it adds multiple flows to the same node. The export file gives the compressed flow file, where only the summed flow per node is given.

**Export restriction data:** Flow division, flow restrictions, and the height of weirs at the start of a pipe are given in the restriction file (section 4.2.3). During the setting up of the network file, WATS can automatically assign restriction to flows according to the link type (section 4.2.3.1). The so modified restriction data can be exported back to a txt file holding the restrictions.

## 5.2 Automatic filling in missing information and checking data validity

It is quite common that network data files have gaps in them, for example that a pipe roughness is missing, a length, or an elevation. Mega-WATS attempts to fill in these gaps based on the information from adjacent pipes. The filling in of missing data and the checking of the validity is done every time the data files are loaded.

Modified pipes can be shown choosing the 'Show modified pipes' on the 'Debug' page (Figure 44). If some such pipes are found, the types of issues encountered are shown by bolding the name, e.g., *Dwstr. X* and *Dwstr. Y* in the given example.

Missing x,y-coordinates of nodes	Searches for another occurrence of the same node and uses the x,y-coordinate of that node If such cannot be found, a best guess is made on where the node might be. In the example of Figure 44, the coordinates of the node 15260001 are missing and have been filled in. Obviously, this is not quite correct, and should be fixed.
Missing pipe length	Calculates the geometric length between upstream and downstream nodes
Missing upstream and downstream pipe elevation	Searches for another occurrence of the same node and uses the elevation of that node. If there are more than one pipe to choose from, then the elevation of the one with the lowest invert is chosen. If slope and length are given and either an upstream or downstream elevation is given, the missing elevation is calculated from this information.
If elevations are missing and have not been found by the previous approach	The slope is set to the default pipe slope which is set in the setup menu (Figure 38). Elevations are calculated based on this slope
Missing diameter, width, and height	Searches for downstream and upstream pipes and assumes those diameters, width, and height for the missing values
If the pipe roughness is missing or below 0.1 mm or above the maximum roughness	Fills in the default roughness (Figure 38)
If the equivalent alkalinity of a corrodible pipe is not given or less than 0.05	Fills in the default equivalent alkalinity (Figure 38)
If slopes differ from what can be calculated from upstream and downstream nodes and pipe length	Slope is re-calculated
If the material is not given	The default material is assumed (Figure 38)
If the pipe shape is not given, or does not equal a shape in the shape file	The default shape is assumed (Figure 38)

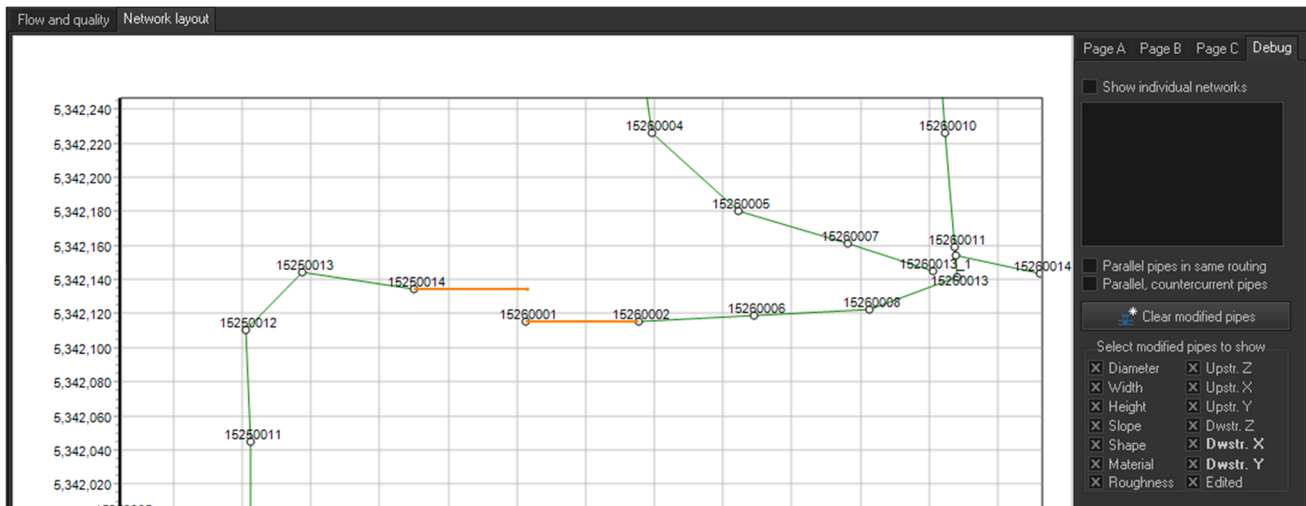


Figure 44. 'Show modified pipes' on the debug page

## 5.3 Loading a network - warnings and errors

### 5.3.1 Problems and information files

When creating a project, Mega-WATS creates two information files and two problem files. These are accessed by the bottoms in the lower left corner of the 'Build a project' menu (Figure 11). These warnings and errors will not hinder the operation of the model but might tell that there are bugs in the network or flow file which maybe should be corrected. Some of the bugs are severe, like the one discussed in section 5.3.3, others less so, for example if a pipe shape is not given, and the pipe instead is treated as circular.

In any case: When setting up a new model, these files should be checked and used in the debugging.

### 5.3.2 Wrong node coordinates

Had the coordinates in the network shown in Figure 38 not been missing, but filled in with zeros, Mega-WATS sees those as true coordinates. This results in the map looking quite wrong (Figure 45). The user must in this case find the missing information and correct it in the network file.

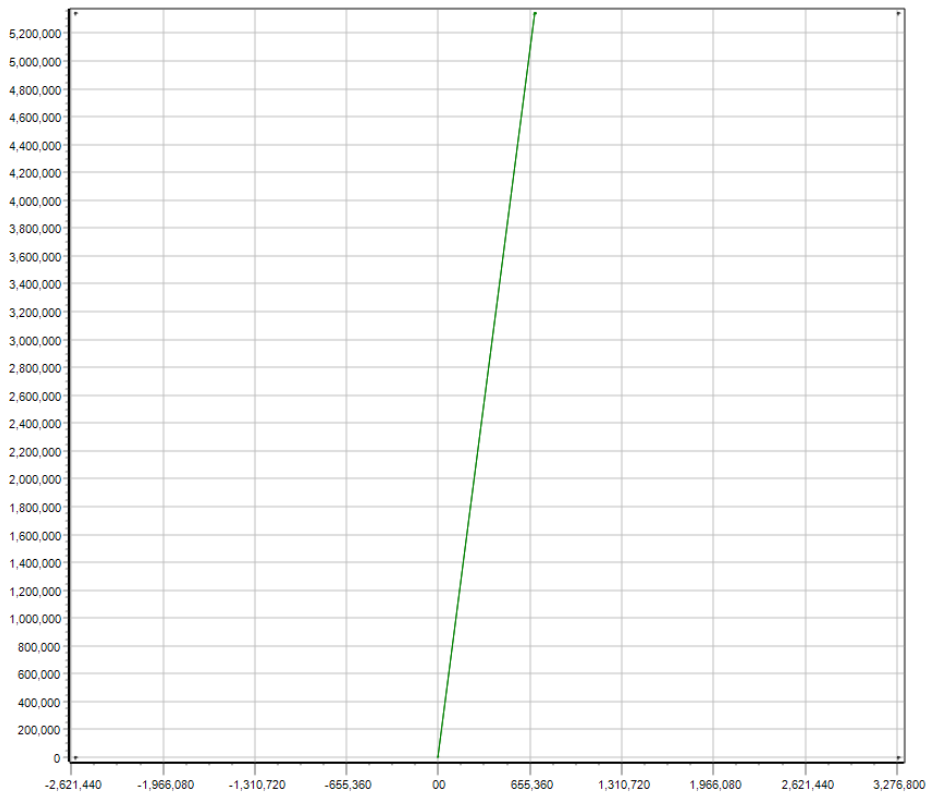


Figure 45. A map where one node has the coordinates (0,0)

### 5.3.3 Nodes with the same names but different coordinates

The same node name can have been assigned different coordinates. Or the other way around: Two nodes which should be different have been assigned the same name but different coordinates. While this is not common, it can happen, and causes quite severe issues for the model. Most often the issue occurs when a larger network is stitched together from several datafiles, and where those datafiles have not used a stringent naming convention for nodes. As Mega-WATS uses nodes to link pipes, this causes the water to be ‘zoomed’ from one part of the network to another.

Figure 46 illustrates such a problem. A node of the name 14460003 is found in both the left and right part of the network. This is an error which leads to water from the right part of the network being ‘zoomed’ to the left part. This causes all downstream calculations to be wrong, as the water from the right part of the network is mixed into the water from the left part.



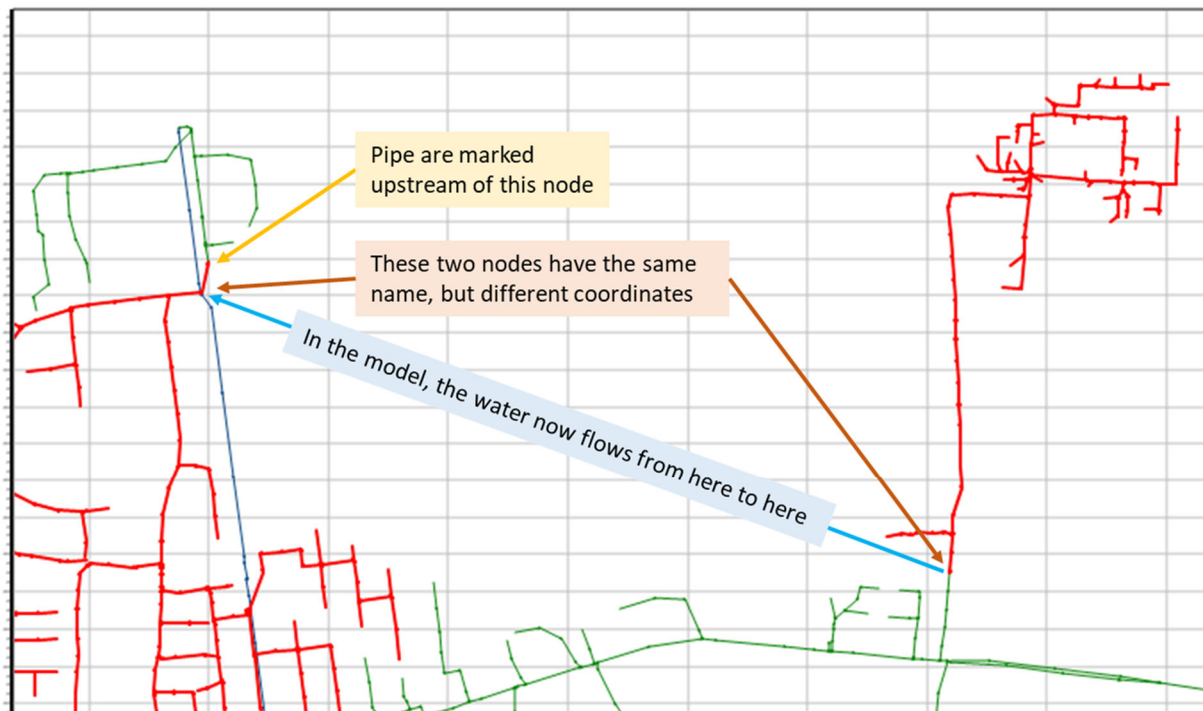


Figure 46. Two nodes have received the same names, but are in different parts of the network

Mega-WATS searches for such errors and reports them in the network problem file (section 5.3.1) as shown in Figure 47. The criterium for two coordinates being different is if their coordinates are more than 0.1 m apart.

```
File
There are issues with the same node having different coordinates. This causes severe errors in the simulations. The pipes are:
14396 and 40211 have different coordinates for the same node: 14460003 - the distance is 2137.41 m
```

Figure 47. Reporting of the error illustrated in Figure 46 in the network problem file

### 5.3.4 Identify circular flow paths

In Mega-WATS, the water flow direction is calculated as being always from the upstream node to the downstream node. This is different from hydrodynamic models, which calculate the flow direction based on water levels (pressure gradients). This means that Mega-WATS is sensitive to the pipes pointing in the right direction. Due to this, one error which the user must check for is 'circular flow paths'. The first step in doing so is to view the network error file for occurrences of the message 'The pipe PipeNameA and PipeNameB have each other's Upstream Nodes as Downstream Nodes'. This will lead to water flowing in an infinite circle. The pipes must be identified, and the erroneous pipe removed from the dataset (or its direction changed).

The pipe error file furthermore will show such errors by the text 'The pipe PipeNameC could not be calculated due to a fatal error in the network. There is probably a circular flow pattern in the network'.

When such an issue is found, the user should access the *Debug page* (right side of the user interphase, Figure 4) and click the *Information on network* button. In the form that appears (Figure 48), click the button *Circular flow paths*. If such exist, they will be highlighted (Figure 49). Circular flow paths must be identified, and their

source removed. In the example shown, the error turns out to be in the western-most part of the network, where the flow runs in an indefinite circle of pipes 52270416, 52270418, and 52270417 (Figure 50). Pipe 52270417 seems unnecessary and removing it from the dataset solves the problem of a circular flow path. It can in some cases be somewhat difficult to identify the issue, but it is crucial that there are no circular flow paths in a network, as these hinder a proper simulation.

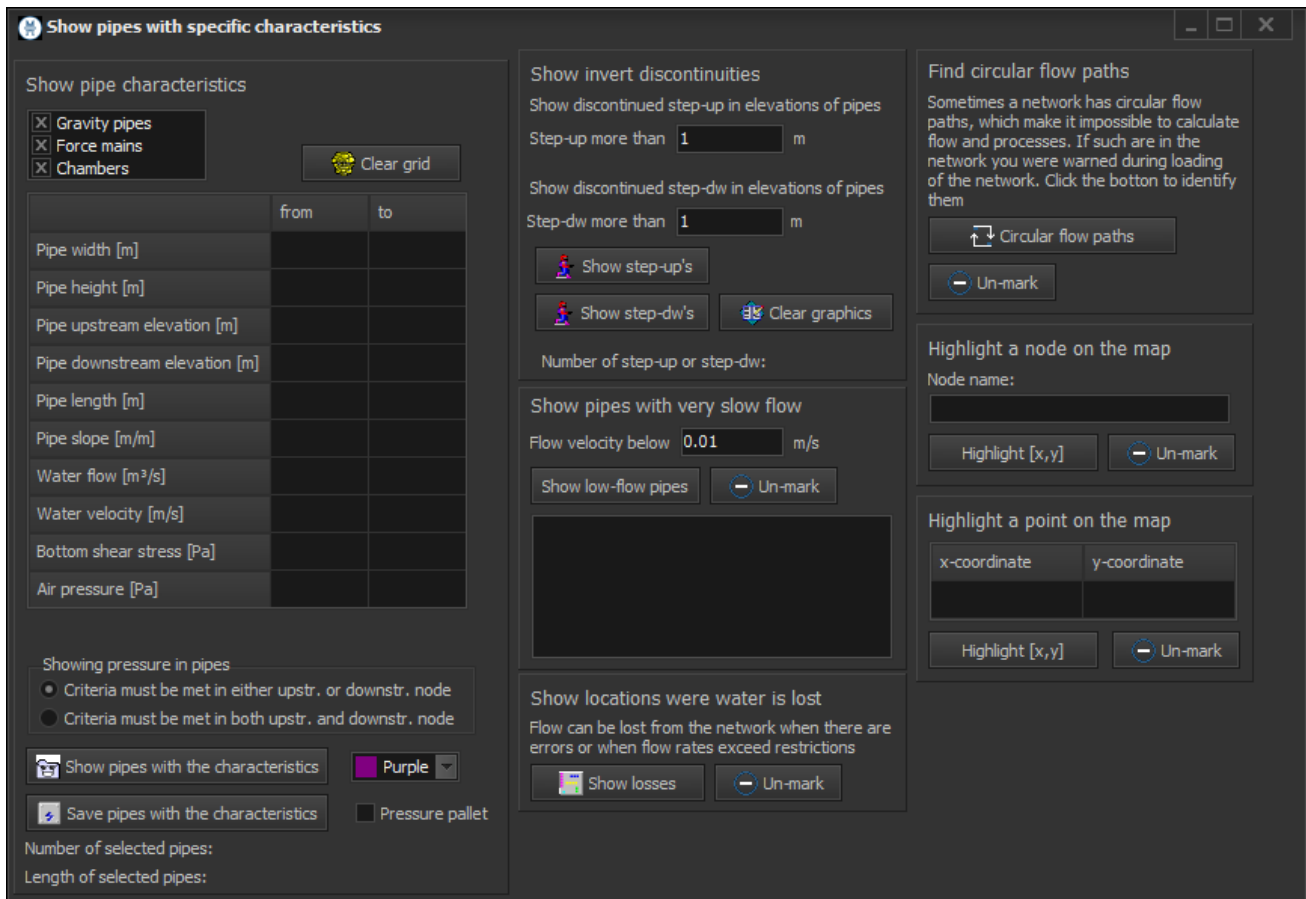


Figure 48. Showing pipes with specific characteristics and issues



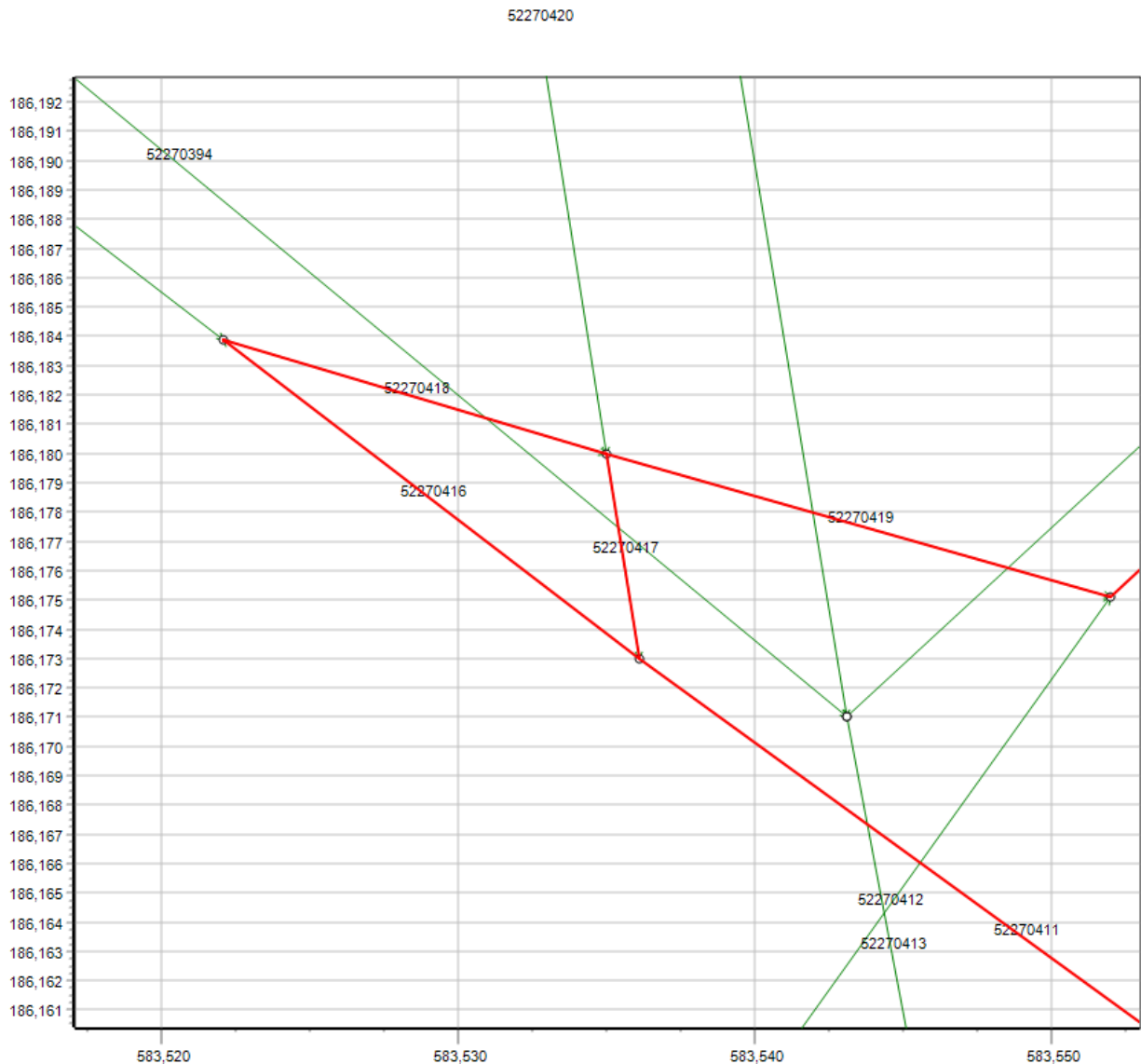


Figure 50. The cause of the circular flow path shown in Figure 49

### 5.3.5 Show pipes with long residence times

Very long residence times, or slow flow velocities, are often caused by errors in the network. Hence, checking for this is part of the debugging. This is done from the *Debug page* (right side of the user interphase, Figure 4) and click the *Information on network* button. In the form that shows (Figure 48), click the button *Show slow pipes*. The criterion for what is a long residence time is set in the edit field *Calculation times above*. Default is 0.1 s, but it can be convenient to use different values.

Figure 51 shows an example of such long residence time, in the concrete case caused by a very low flow in an upstream pipe. This pipe alone requires 3.68 s calculation time out of the 45.6 s used to calculate the whole network of 33215 pipes with a total length of 1633 km. Moving the flow entering the upstream node one tier downstream would solve this issue and save nearly 4 s of calculation time.

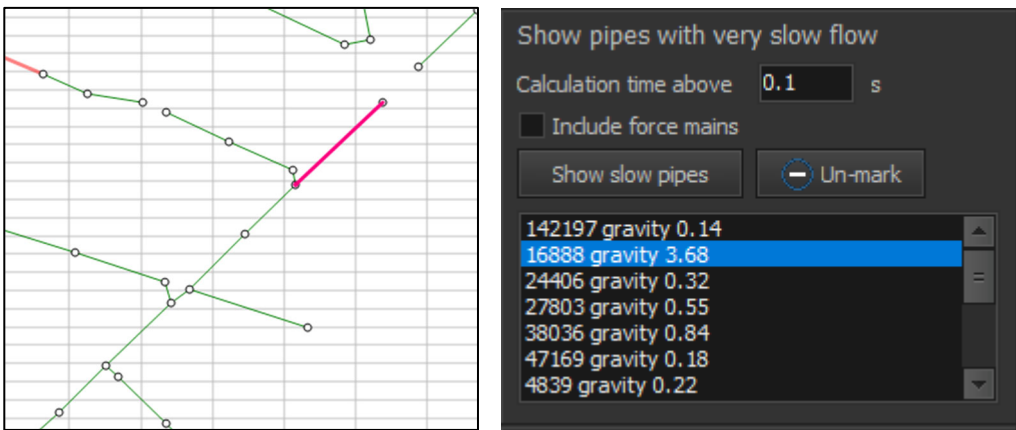


Figure 51. Pipes with low flow velocity

## 5.4 Show individual networks

For one reason or another, networks might not be connected. These issues can be identified by checking the *Show individual networks* checkbox on the *Debug* page. An example of this is shown in Figure 52. For identifying individual networks, the *Show discharge points* checkboxes on the *Show B* page may also come in handy. One can choose to view all discharge points or only those that hold flow.

Some individual networks are natural for Mega-WATS, namely those that occur when the network conversion has identified an overflow (section 4.2.3). They will typically consist of one or a few pipes that do not hold flow. Other natural individual networks occur if both stormwater and wastewater pipes have been included in the network. Or when there for other intentional reasons for more than one separate network.

Other errors occur because the link between two parts of the network is incorrect, for example a missing pipe or a wrongly named pipe node. These have to be identified and fixed.

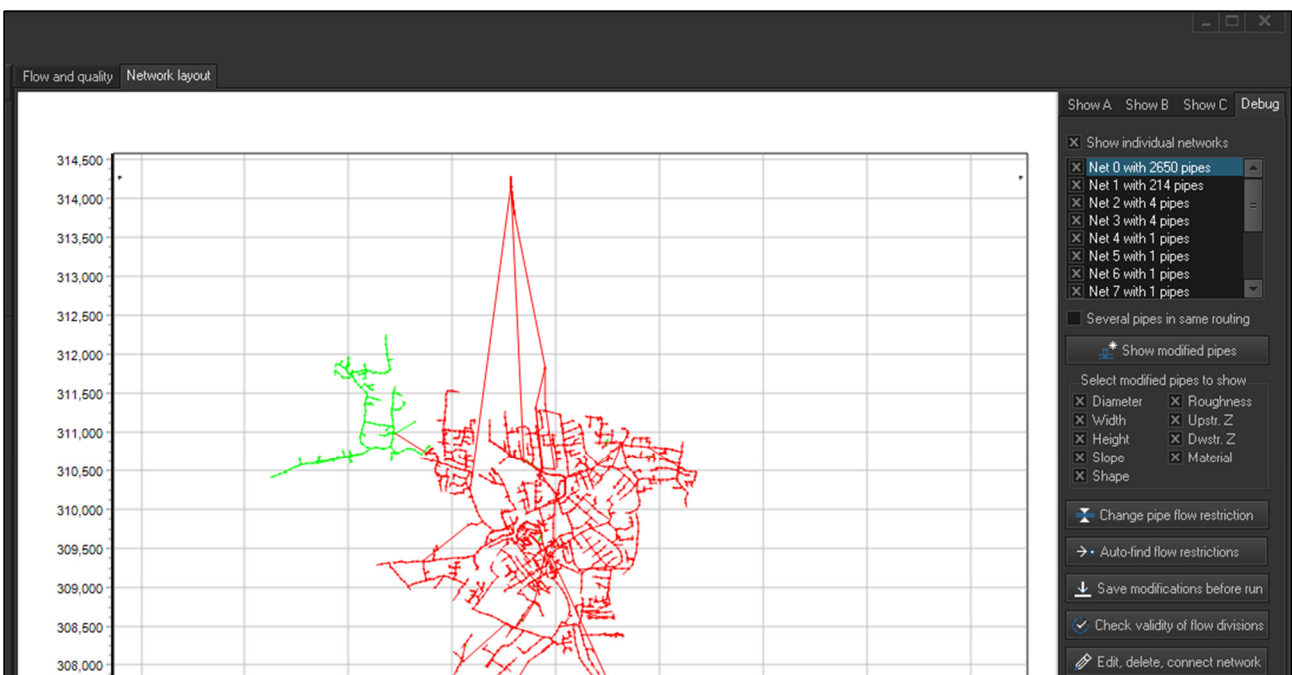


Figure 52. Identifying individual networks

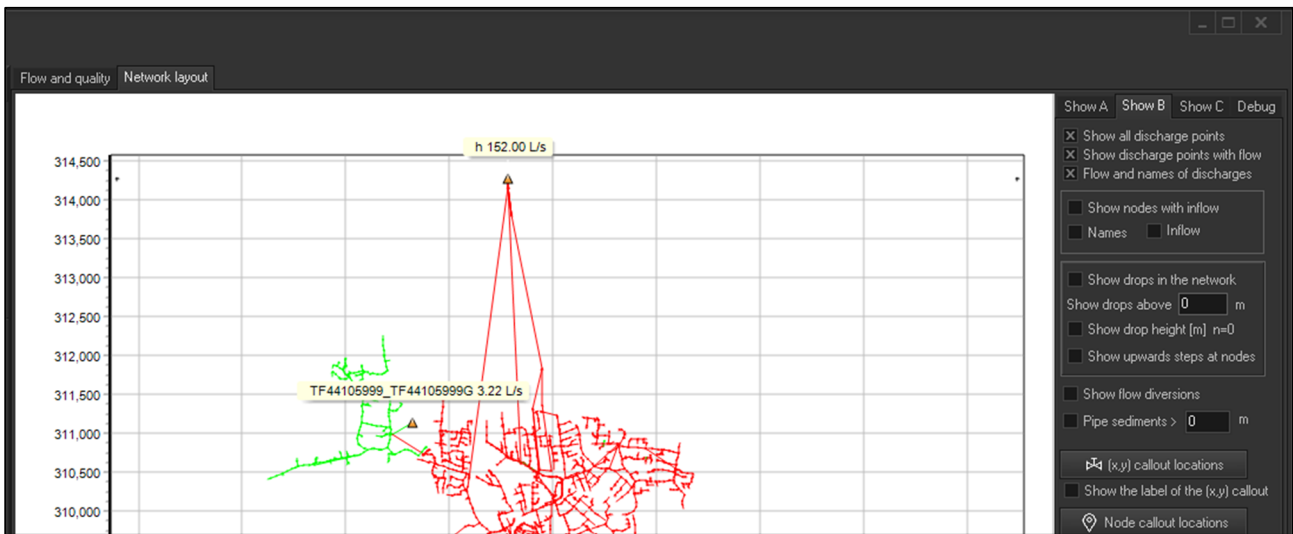


Figure 53. Show discharge points with flow

## 5.5 Flow direction

Mega-WATS has a pre-defined direction of flow in a pipe: The water always flows from the upstream node to the downstream node. The direction of the flow can be shown by clicking the *Indicate flow direction* checkbox on the *Show A* page. An example is given in Figure 54.





Figure 54. Indicate the direction of flow in the network

## 5.6 Flow paths

Flow paths is an important tool to get information on the processes in the pipes and errors in the network. A path is created by choosing a *From pipe* and *To pipe*, then pressing the blue arrow lowest on *Page A* (Figure 55).

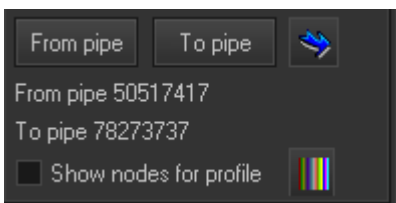



Figure 55. Selecting a flow path



The nodes of a flow path can be shown as dashed lines by checking the Show nodes for profile checkbox. Their color can be set in the color-selection dialog. 

After having selected the flow path, the path turns red (Figure 56) and the pipe box listing information on the pipes shows some specific information for the flow path, namely start and end pipe, travel time for water and air, and water and air volumes in flow path. Choosing a pipe removes this information and shows instead the information for the pipe in question. To re-show it, the blue arrow has to be clicked again.

An important tool to find errors is the flow path. Flow paths allow the user to plot water quality parameters, pipe geometry, and flow depth along from any selected upstream node to any downstream node. Consider, for example, the part of a network shown in Figure 56 with its corresponding pipe profile shown in Figure 57. The pipe around position 250 m has backwater because its downstream elevation is about 0.1 m lower than the upstream elevation of the downstream pipe. This is probably a data error in the network file. All the small drops of a few centimeters downstream here of are probably also data errors and not the real pipe invert.

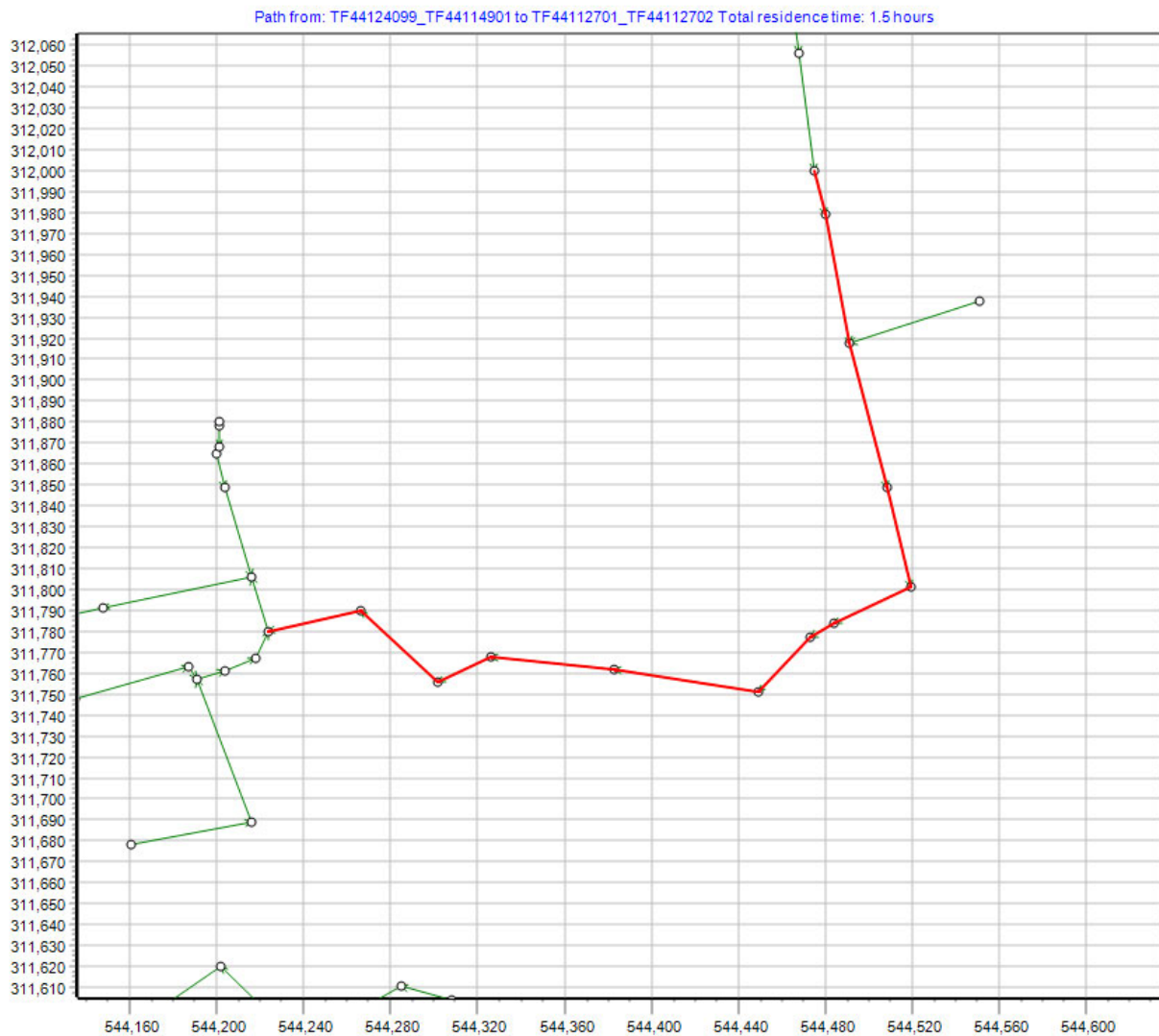


Figure 56. A flow path in part of a network

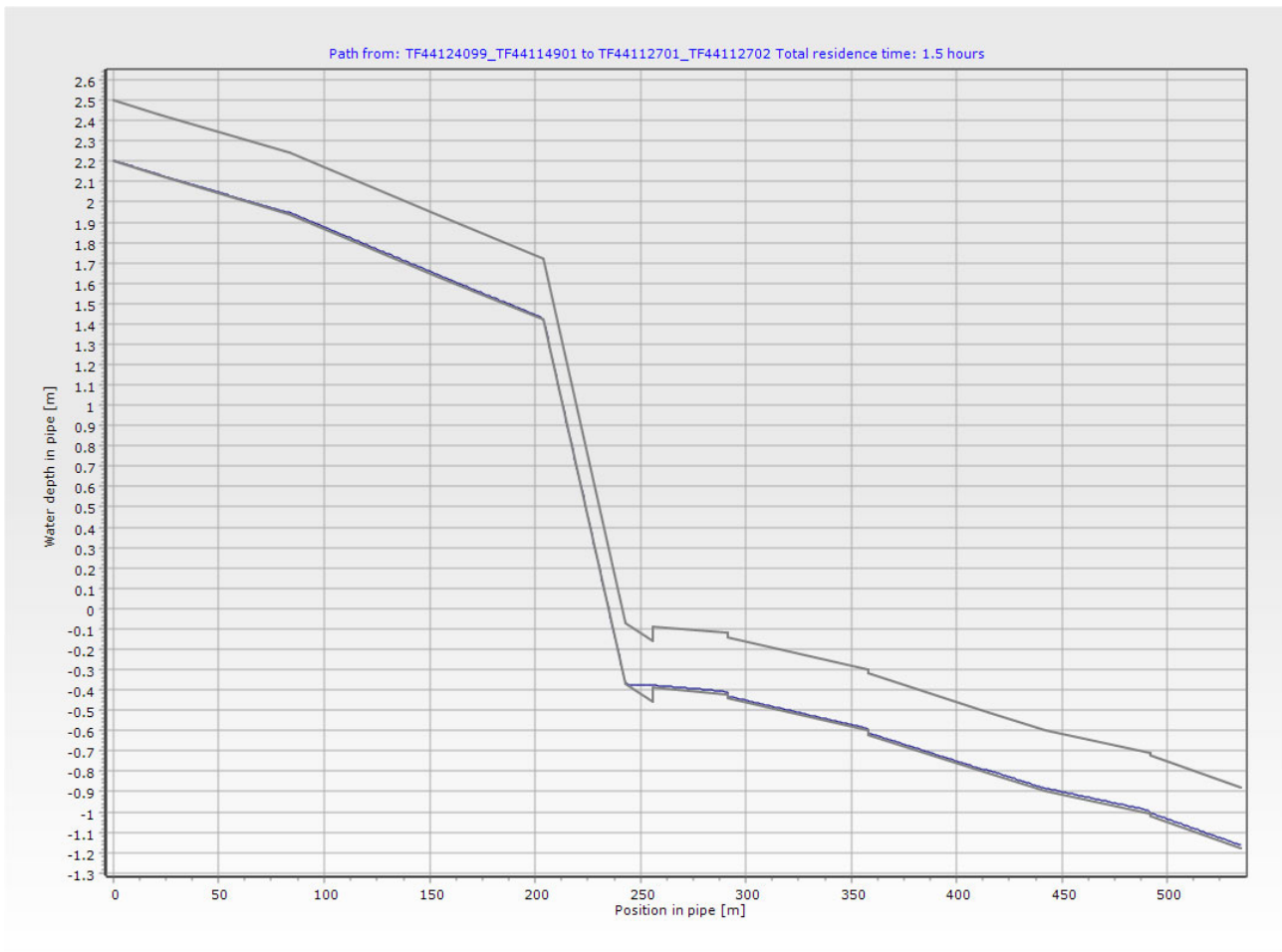


Figure 57. The pipe profile corresponding to the flow path of Figure 56

### 5.6.1 Plotting flow path data

Data on flow and water quality can be exported at the same resolution as the model simulations (typically approx. 1 m). One can access the page for the export from the main form menu: *Output* → *Write flow path data to text file*). The form allows exporting a variety of parameters by checking the ones needed ().

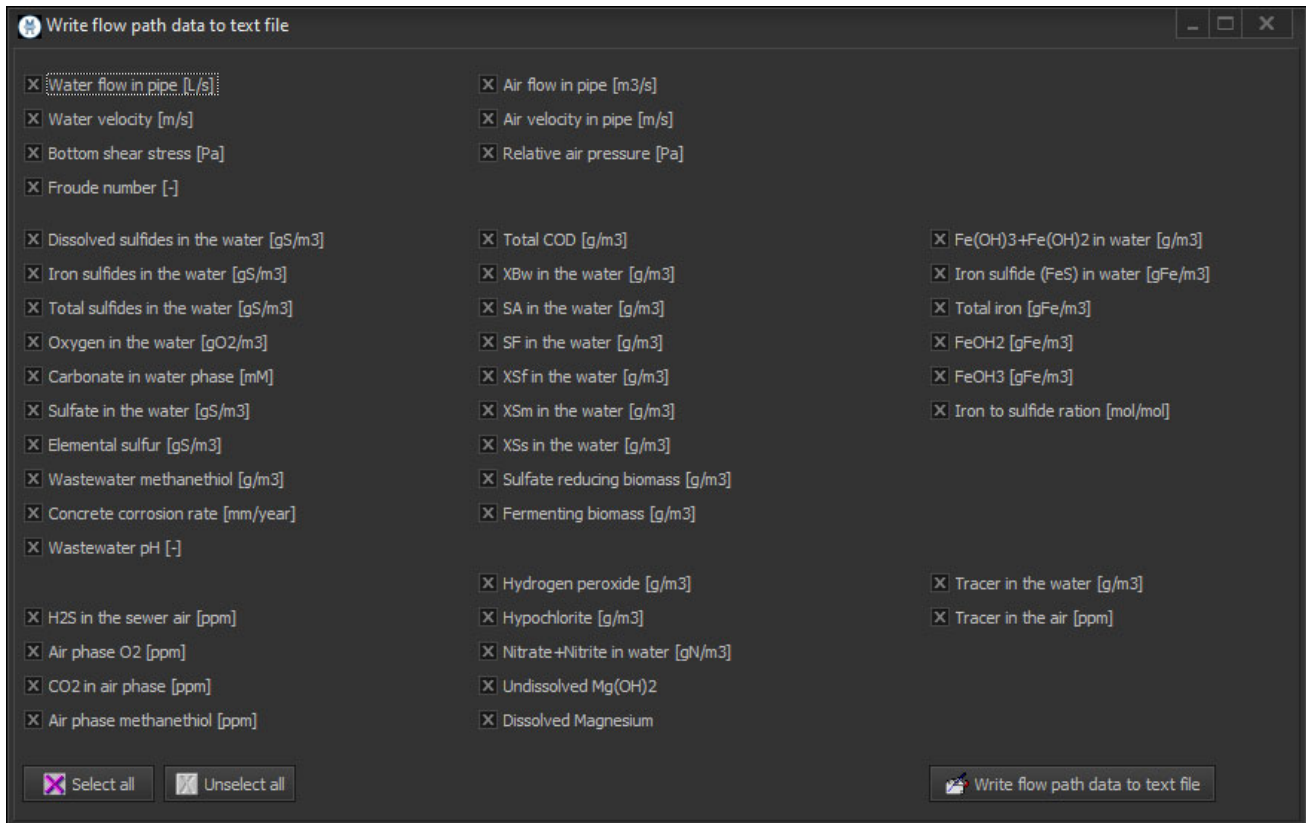


Figure 58. Writing data from a flow path to a text file

## 5.7 Identifying wrong inverts

### 5.7.1 Show negative slope

Pipes may have wrong inverts for various reasons. Many of these errors have little impact on a hydrodynamic model, the purpose of which is to simulate wet weather. However, they can have severe impacts on the validity of a dry weather process model and these errors must hence be identified and removed. Consider, for example, the pipe shown in Figure 59. The water flows towards the left and there are several negative slopes (check the *Pipes with negative slope* checkbox on the *Show A* page). Viewing the flow path (Figure 60) there are obvious issues with the pipe profile. This would not have been an issue in a hydrodynamic model which relies only on invert levels, not on flow directions, but for Mega-WATS it constitutes a problem. This issue causes very long residence times, which again result in very high sulfide concentrations, which do not occur in the real network. Other examples are shown in Figure 61 and Figure 62, which identify a somewhat weird invert which probably is an error in the network file.

A further quite common issue is that upstream and downstream pipes can have been swapped, leading to negative slopes. This is easily solved by swapping the upstream and downstream pipe nodes (Section 5.8.6).

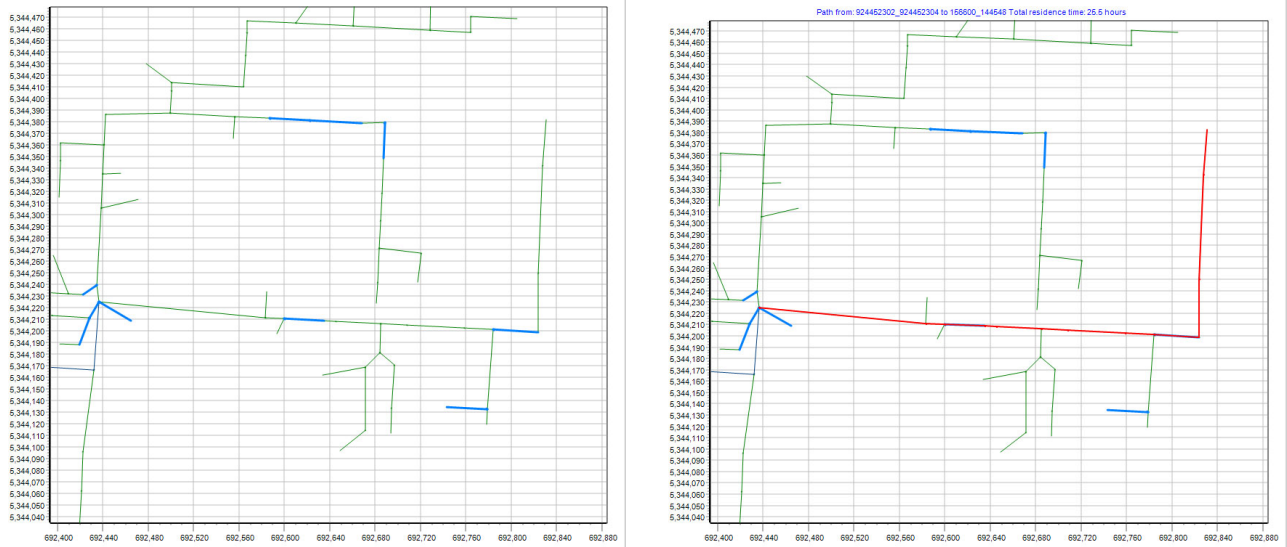


Figure 59. Pipe marked as having negative slope (left). Flow path including the negative sloping pipe (right)

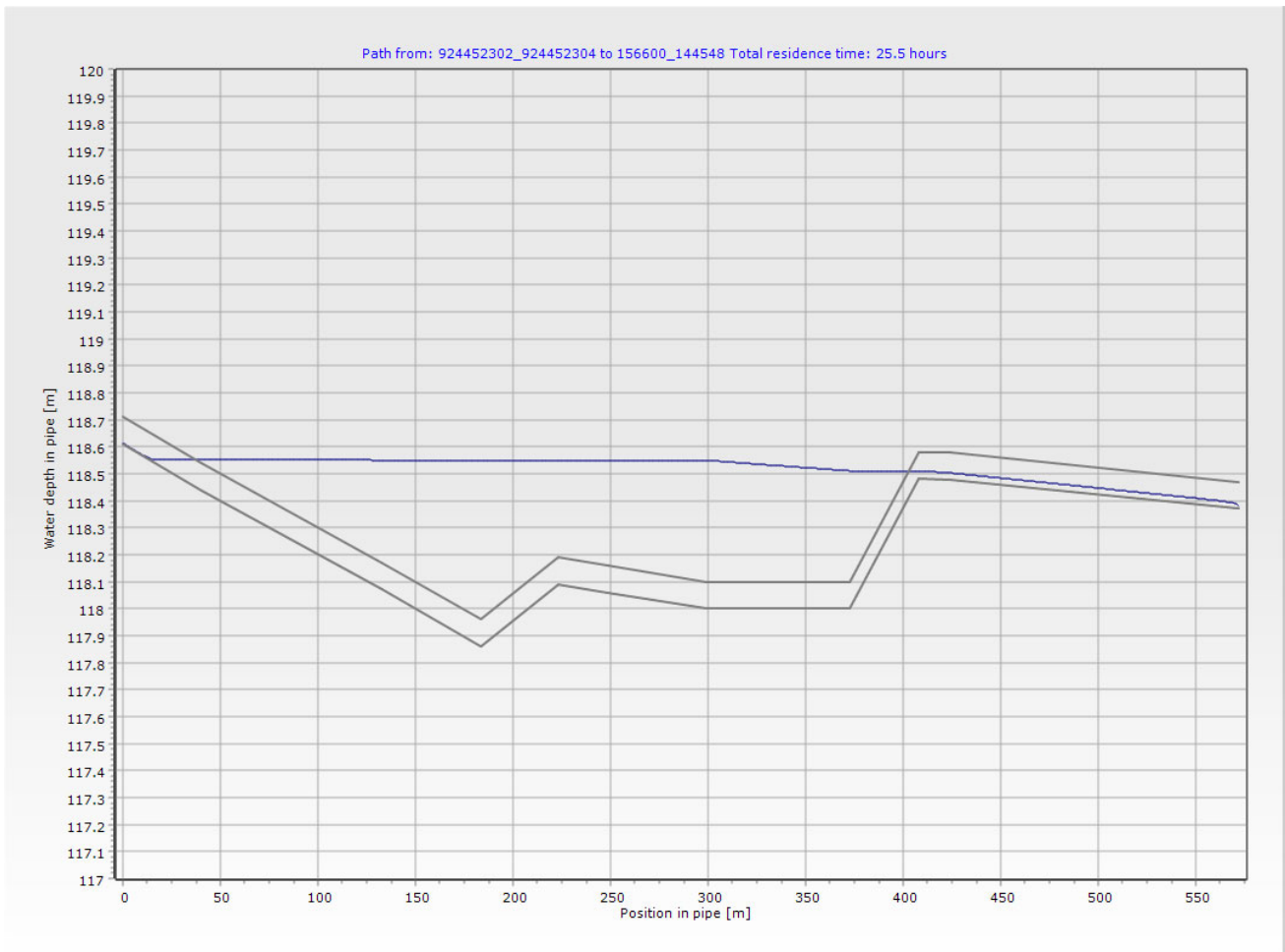


Figure 60. Pipe inverts corresponding to the flow path of Figure 59

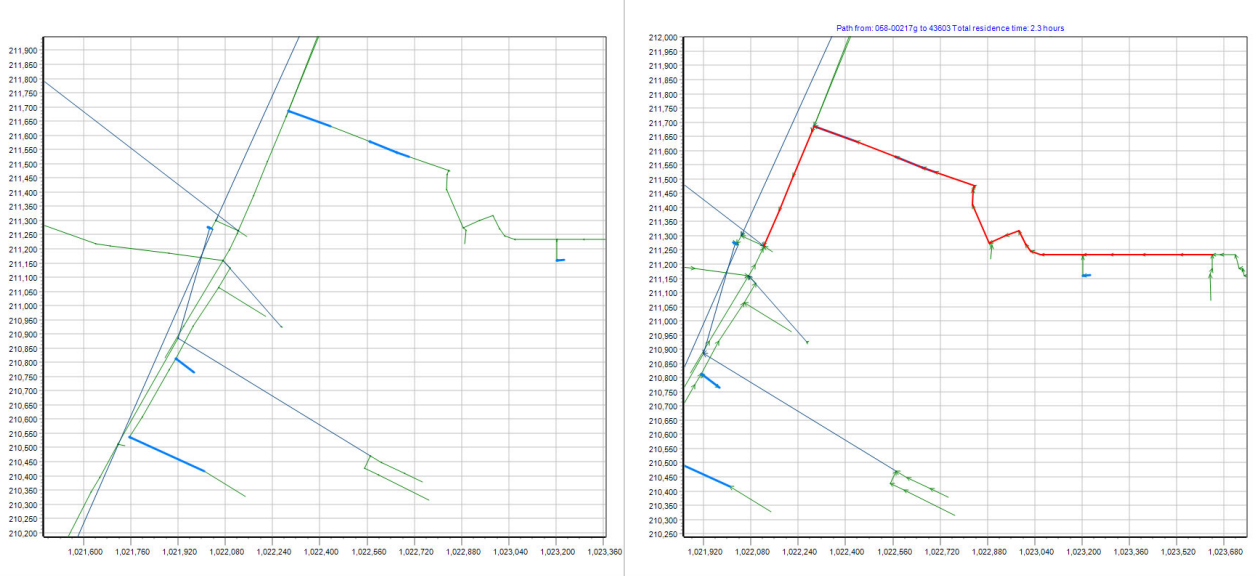


Figure 61. Pipe marked as having negative slope. Flow path including the negative sloping pipe

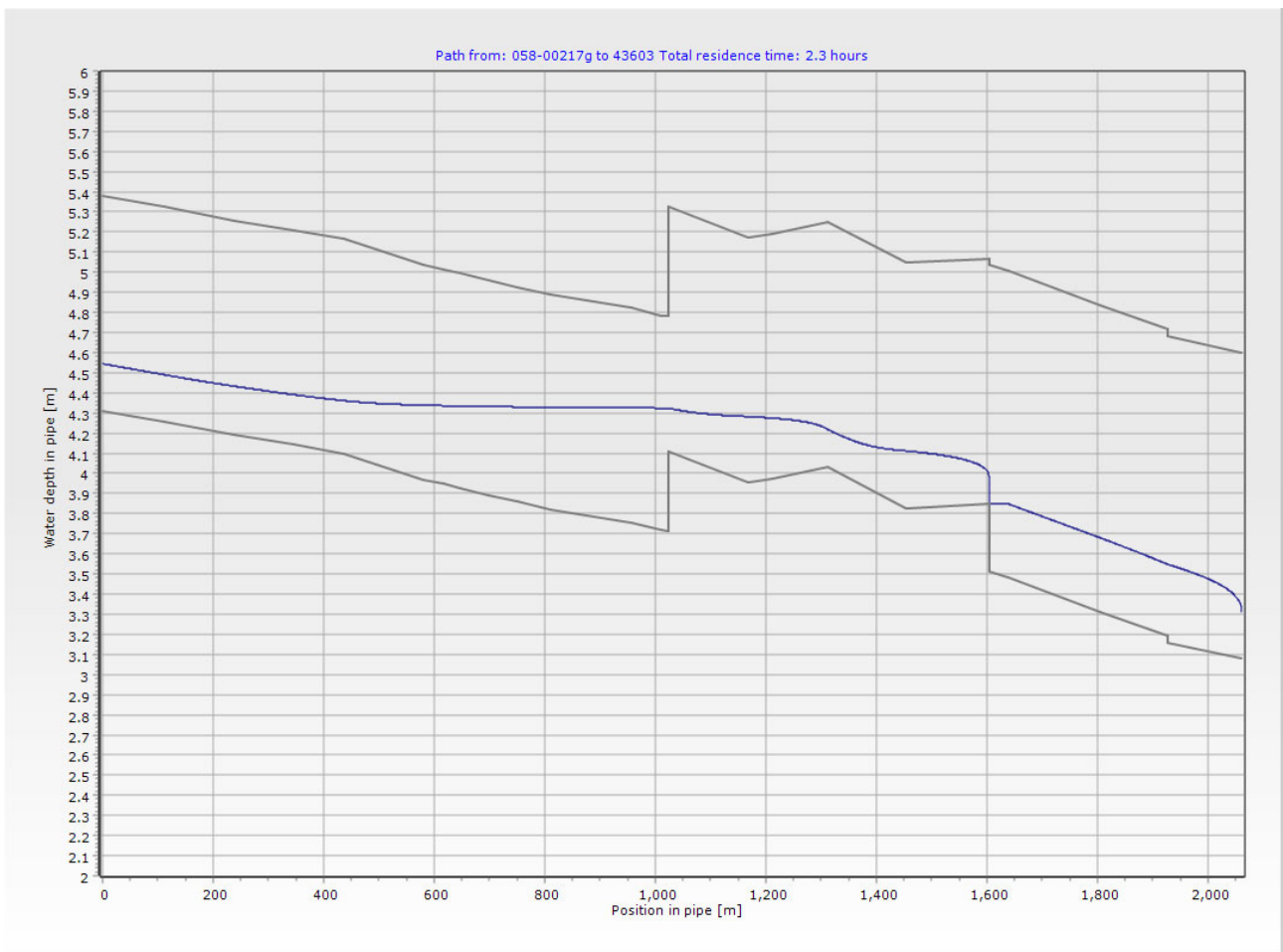


Figure 62. The invert of the flow path shown in Figure 61

### 5.7.2 Show pipe steps-up and drops

Another way to identify issues with the invert is to use the *Show upwards steps* facility. This can be done either by checking the *Show upwards steps at nodes* checkbox on the *Show B* page, or in the edit pipes and nodes menu (section 5.8) or on *Page B* of the main menu.

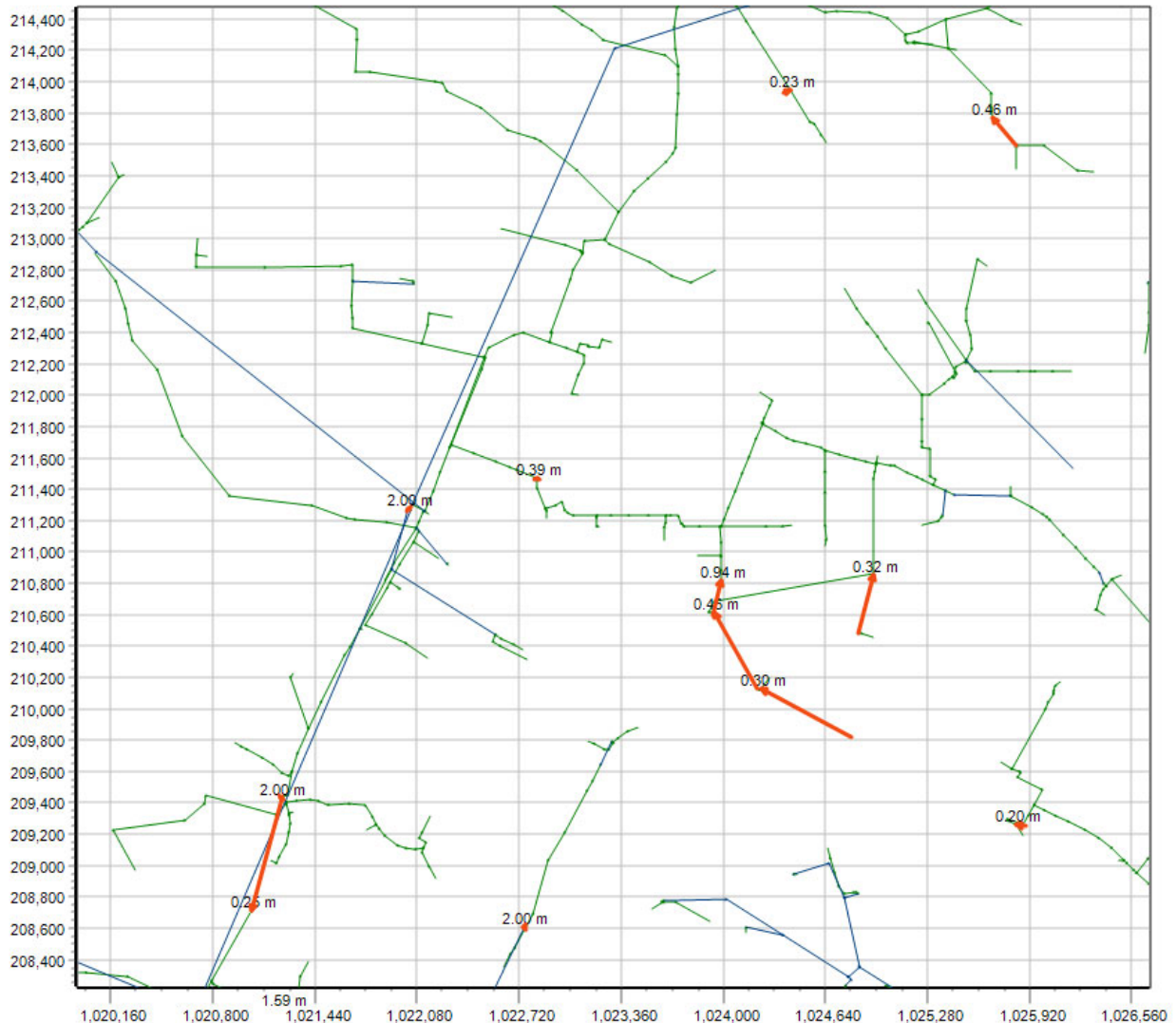


Figure 63. Drops in a network

Drops are often true elements of a sewer network but can also be errors in the pipe inverts (Figure 63). Drops can be shown either by checking the ‘Show drops in the network’ checkbox on the *Show B* page, or in the edit pipes and nodes menu (section 5.8).

### 5.7.3 Flow splitting / divisions

Most of the time a sewer network is a branched system where many small pipes joint into ever-bigger pipes, i.e., a tree structure. However, flows can also diverge. Diverging flow can be shown by checking the *Show flow divisions* checkbox on the *Show B* page. An example of such visualization is shown Figure 64, where also



the flow direction and the nodes are shown. Most likely the diversions are real, however, sometimes they are not. In such case, the flow should be restricted from the pipes which are not supposed to hold flow (Section 4.2.3).

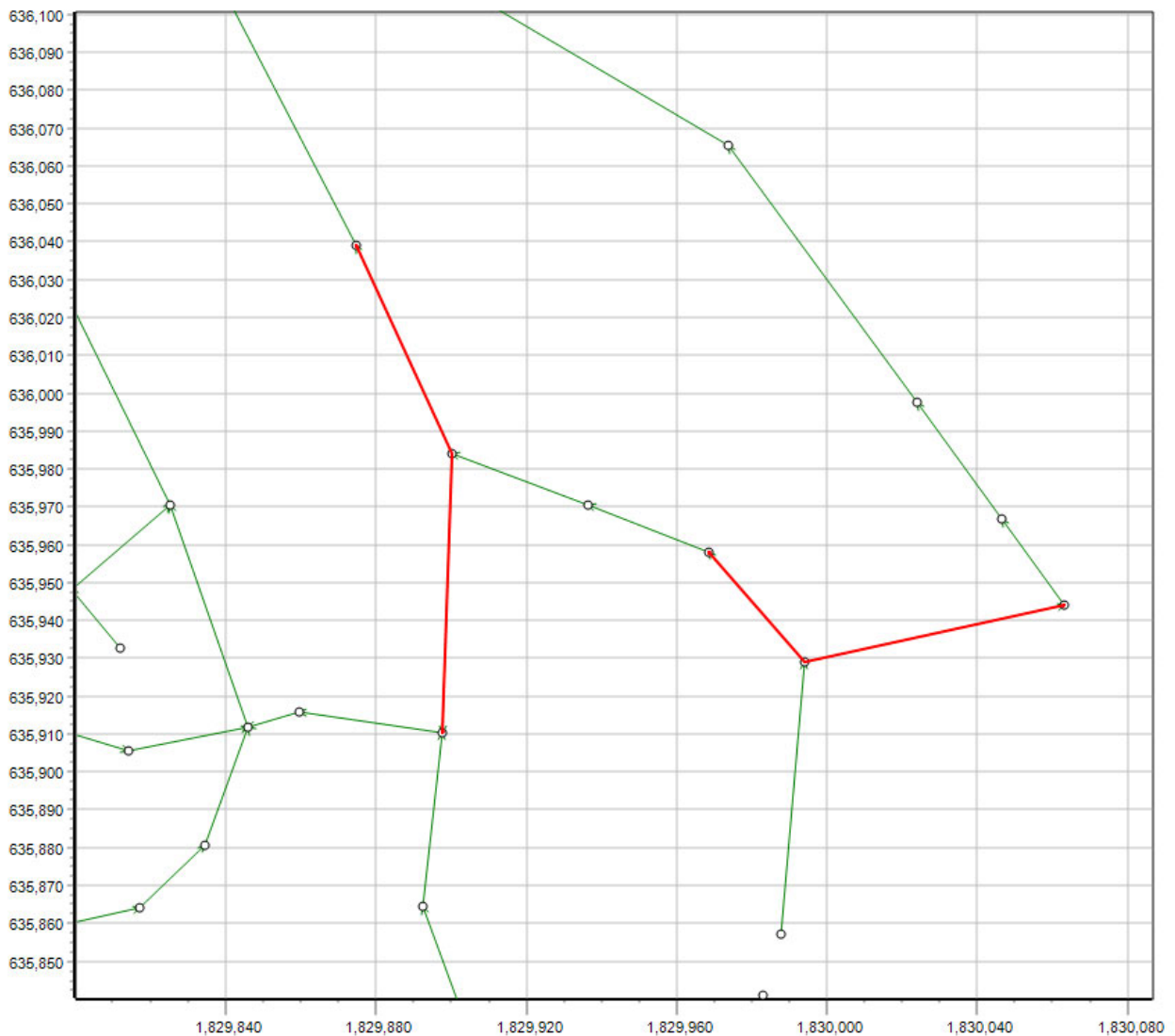


Figure 64. Indicating flow divisions

## 5.8 Edit the network layout

Usually, a network imported from a hydrodynamic model or similar has several issues when it is loaded into Mega-WATS. Some of these are also present in the original model, while some are due to small differences between the requirements of Mega-WATS compared to those of the hydrodynamic model. These must be identified and corrected. This can either be done in the hydrodynamic model or in Mega-WATS. In general, the first is preferable, but this is not always possible, for one reason or another. Hence Mega-WATS has several routines that allow modifying the network in the GUI (i.e., Graphical User Interface).



The network editing routines are accessed from the *Debug* page, the button *Edit, delete, connect network*, producing the form shown in Figure 65.

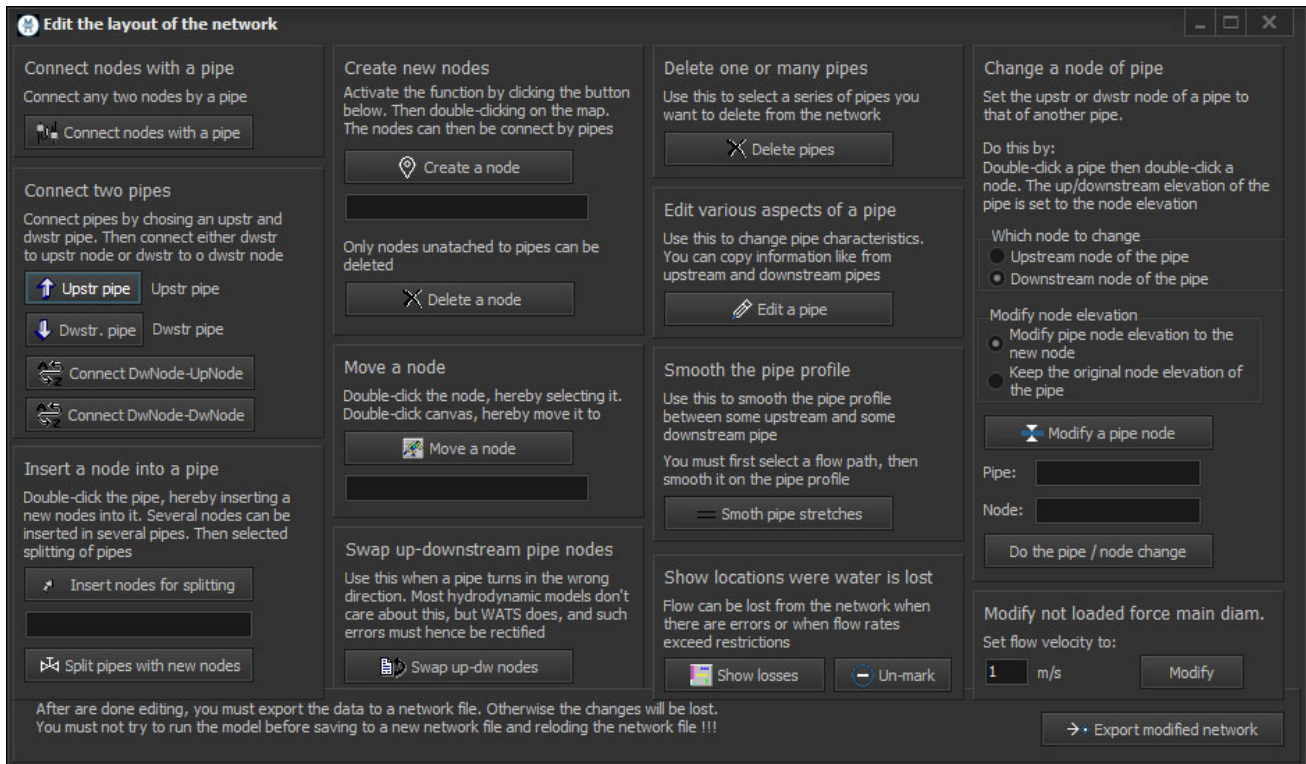


Figure 65. *Edit, delete, connect network* form

Note that there is no option to ‘undo’. Hence one must *Export modified network* at reasonable intervals to avoid losing completed work (Section 5.9.1). When editing the network, the modified pipes can be shown in the export file by selecting the *Network modifications during import* radio button (Figure 73).

### 5.8.1 Connect nodes with pipes

There are several ways of creating links in the network. One is to connect two nodes with a pipe. The nodes can either be existing, or nodes one creates using the *Create new nodes* option (Section 5.8.5).

First click the *Connect nodes with a pipe* button, which will show a new form (Figure 66).

The map will now show all nodes in the network (it checks the *Show nodes* checkbox of the page *Show A*, Section 3.1).

1. Open the *Edit, delete, connect network* form
2. Click the upstream node on the map
3. Click the *Upstr node* button
4. Click the downstream node on the map
5. Click the *Dwstr node* button

The map now indicates which nodes were selected (Figure 67), and the *Connect nodes by pipes* form now is populated with pipe information (Figure 68). If there are more than one upstream or downstream pipe of the nodes, these can be selected to inherit information.

Modify the pipe (the middle grid termed *Pipe joining the nodes* as you see fit, chose whether the pipe is gravity, force main, or chamber, and so on. When satisfied, click *Create the new pipe* which then appears on the map.

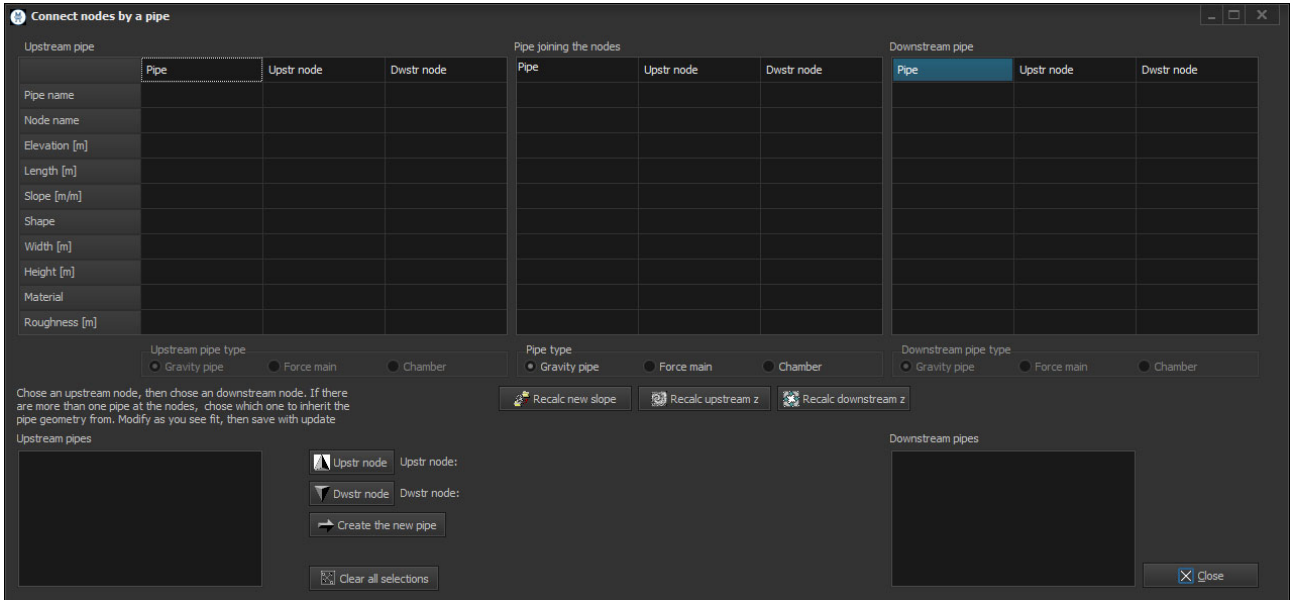


Figure 66. Connect nodes by a pipe form

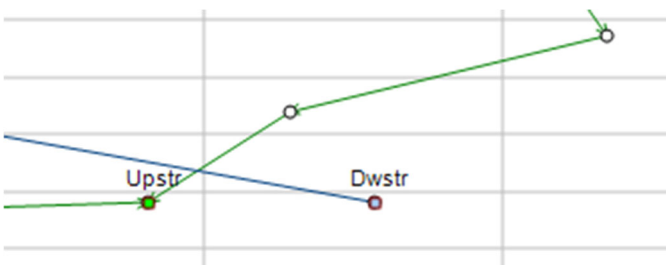
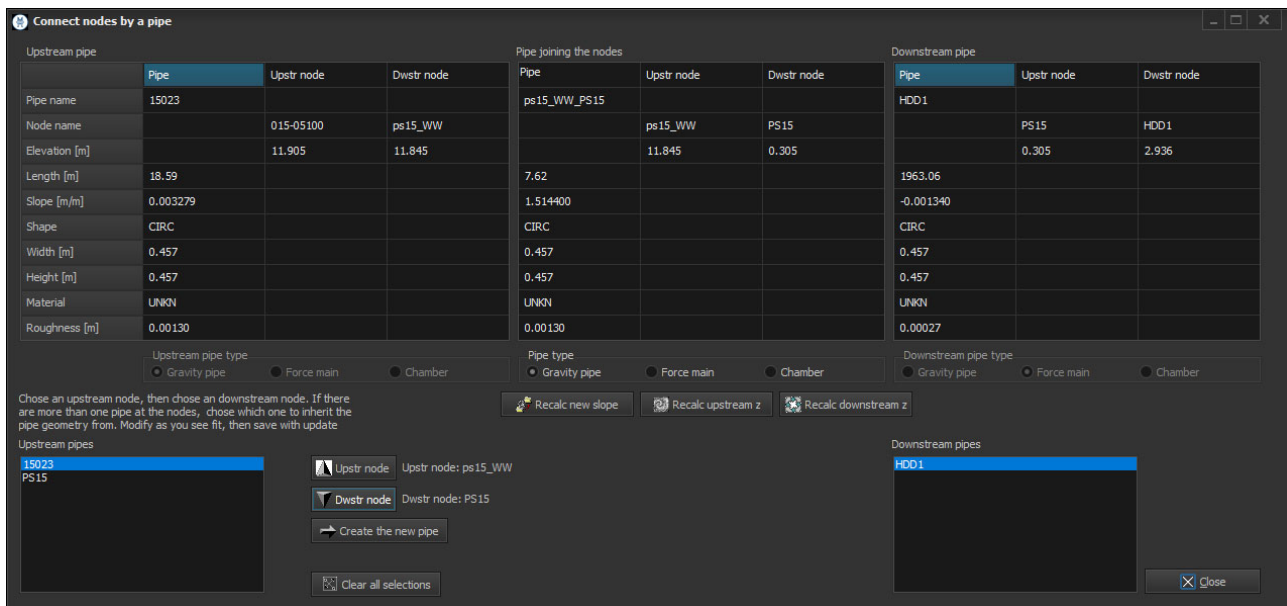


Figure 67. Connecting nodes by pipes: Choosing upstream and downstream nodes, let the nodes be marked on the map



Upstream pipe				Pipe joining the nodes			Downstream pipe		
Pipe	Upstr node	Dwstr node		Pipe	Upstr node	Dwstr node	Pipe	Upstr node	Dwstr node
Pipe name	15023			ps15_WW_PS15			HDD1		
Node name		015-05100	ps15_WW		ps15_WW	PS15		PS15	HDD1
Elevation [m]		11.905	11.845		11.845	0.305		0.305	2.936
Length [m]	18.59			7.62			1963.06		
Slope [m/m]	0.003279			1.514400			-0.001340		
Shape	CIRC			CIRC			CIRC		
Width [m]	0.457			0.457			0.457		
Height [m]	0.457			0.457			0.457		
Material	UNKN			UNKN			UNKN		
Roughness [m]	0.00130			0.00130			0.00027		

Figure 68. Connect nodes by a pipe form, populated with node information

### 5.8.2 Connect two pipes with another pipe

Another way to connect to pipes is by choosing an upstream pipe and a downstream pipe and connecting them.

- Open the *Edit, delete, connect network* form.
- Chose an upstream pipe on the map
- Click the *Upstr pipe* bottom.
- Chose a downstream pipe
- Click the *Connect to DwNode-Upnode* button if you want the downstream node of the upstream pipe (end of pipe) to be connected to the upstream node of the downstream pipe (start of pipe)
- Click the *Connect to DwNode-Dwnode* button if you want the downstream node of the upstream pipe (end of pipe) to be connected to the downstream node of the downstream pipe (end of pipe)

### 5.8.3 Divide a pipe into a series of shorter pipes

In several cases, one is interested in dividing a pipe into a series of shorter pipes, for example, when inserting nodes into a force pipe main for purposes of representing air release valves.

- Open the *Edit, delete, connect network* form.
- Click the *Insert nodes for splitting* button
- Double-clicking on a pipe inserts a node at the clicked position
- Repeat this till the desired number of nodes have been inserted
- Finalize the operation by clicking the *Split pipes with new nodes* button

The length of the two pipes is calculated as the geometrical distance between the new nodes divided by the length of the original pipe. In other words, the sum of the lengths of the new pipes equals the length of the original pipe.

#### 5.8.4 Move a node

In several cases, one wants to move a node, for example after having divided a pipe.

- Open the *Edit, delete, connect network* form.
- Click the *Move a node* button
- Double-click the node you want to move
- Double-click on the canvas where the node shall be placed

The length of the new pipe segments is calculated as the geometrical distance between the nodes.

Upstream and downstream node elevations are maintained, and a new slope calculated.

#### 5.8.5 Create new nodes

When modifying the network, it sometimes can be necessary to create a new pipe. One way is to create one or several new nodes and then connect them with pipes.

- Open the *Edit, delete, connect network* form.
- Click the button *Create a node*.
- Modify the default node name. Make sure that the node name is not already in use!
- Double-click where the node should appear
- Upon having added the needed number of nodes, connect them by pipes as discussed in Section 5.8.1

Nodes which are not attached to any pipe (i.e., created by the process above) can be deleted from the network using the *Delete nodes* button.

#### 5.8.6 Swapping upstream and downstream nodes

The pipe might have a wrong flow direction because its upstream and downstream nodes were swapped in the dataset. While this is of no importance for hydrodynamic models, it matters for Mega-WATS. Hence the flow direction of such pipes should be swapped.

- Open the 'Edit, delete, connect network form'
- Select a pipe
- Press the *Swap up-dw nodes* button

#### 5.8.7 Change the node of a pipe to that of another pipe

A disconnected system, or a system which is incorrectly connected, can also be modified by changing the upstream or downstream node of a pipe to that of another pipe. The procedure is described in some detail on the left part of the *Edit, delete, connect network* form.

### 5.8.8 Smooth the pipe profile

Pipe elevations are often experiencing data issues where there are many small drops in the network file, which are unlikely to be real. Figure 69 gives such example, where there are many small drops of some centimeters. These can be smoothed as follows:

- Select the flow path of interest
- Open the *Edit, delete, connect network* form
- Press the *Smooth pipe stretches* button
- The form *Smooth pipe profiles* opens, giving guidance on how to do it
- There must be at least three pipes in the 'smoothing stretch'
- Smoothing can be done repeatedly

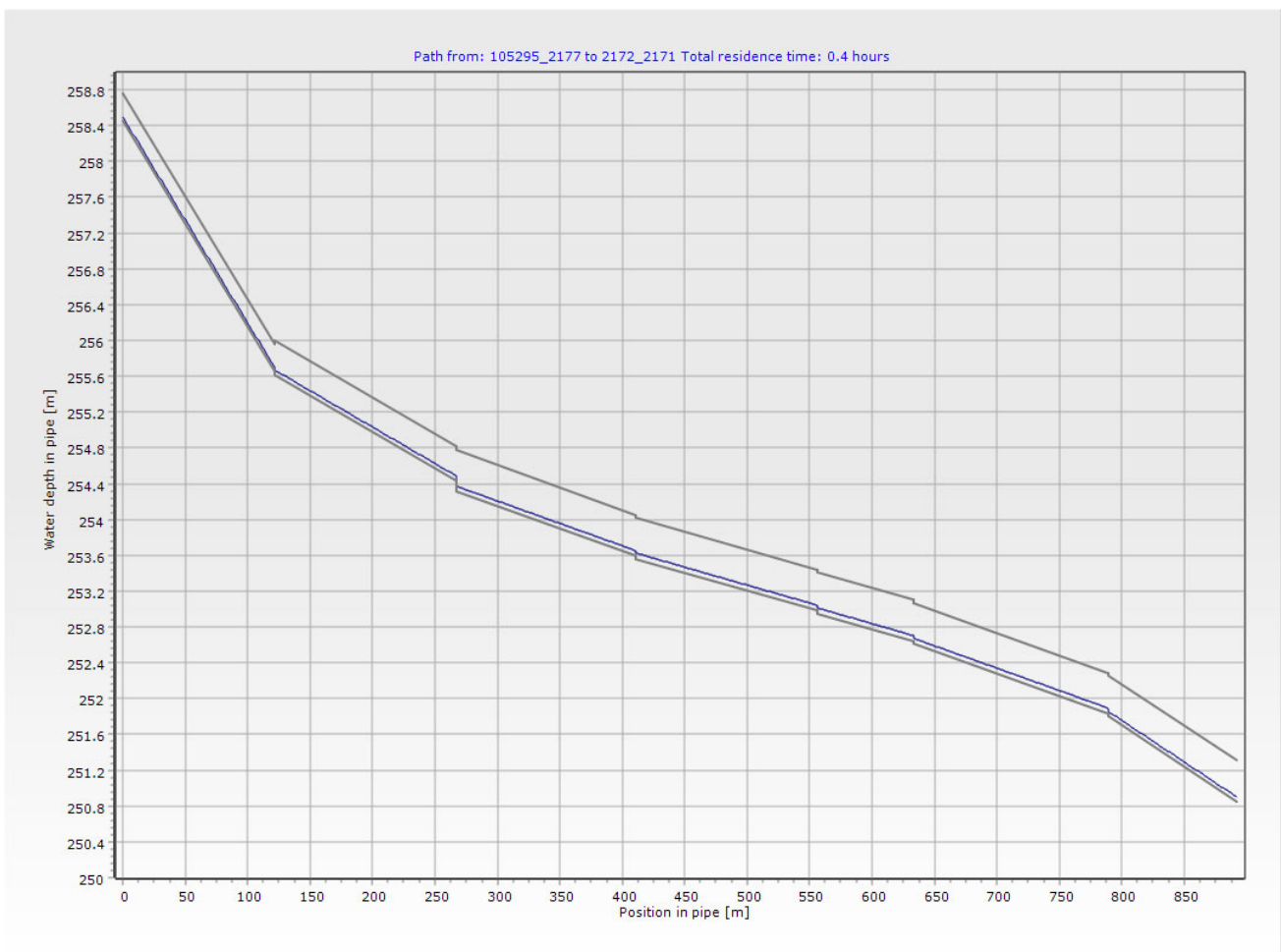


Figure 69. A pipe profile with many small drops

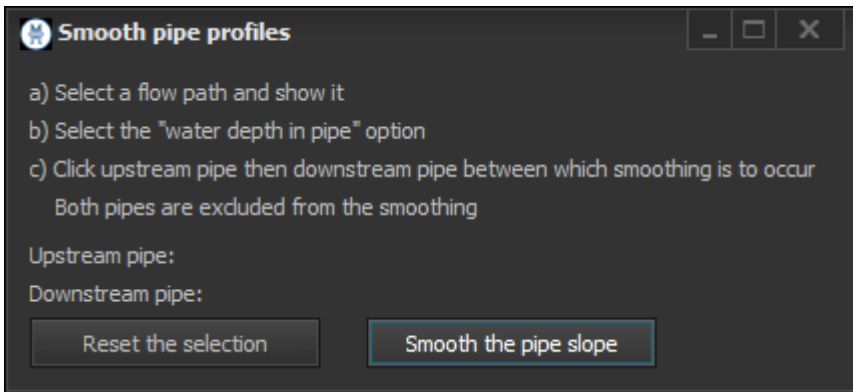


Figure 70. Smooth pipe profiles form

### 5.8.9 Change pipe elevations and other pipe characteristics

Another way to modify the flow profile is to use the Edit a pipe form. This opens the menu shown in Figure 71. Now double-click on the pipe in the map which needs editing, and the form populates (Figure 72). In the example, the pipe 4210\_4209 has three upstream pipes and one downstream pipe. Parameters such as elevation can now be changed either manually, or by using the various buttons in the lower part of the form.

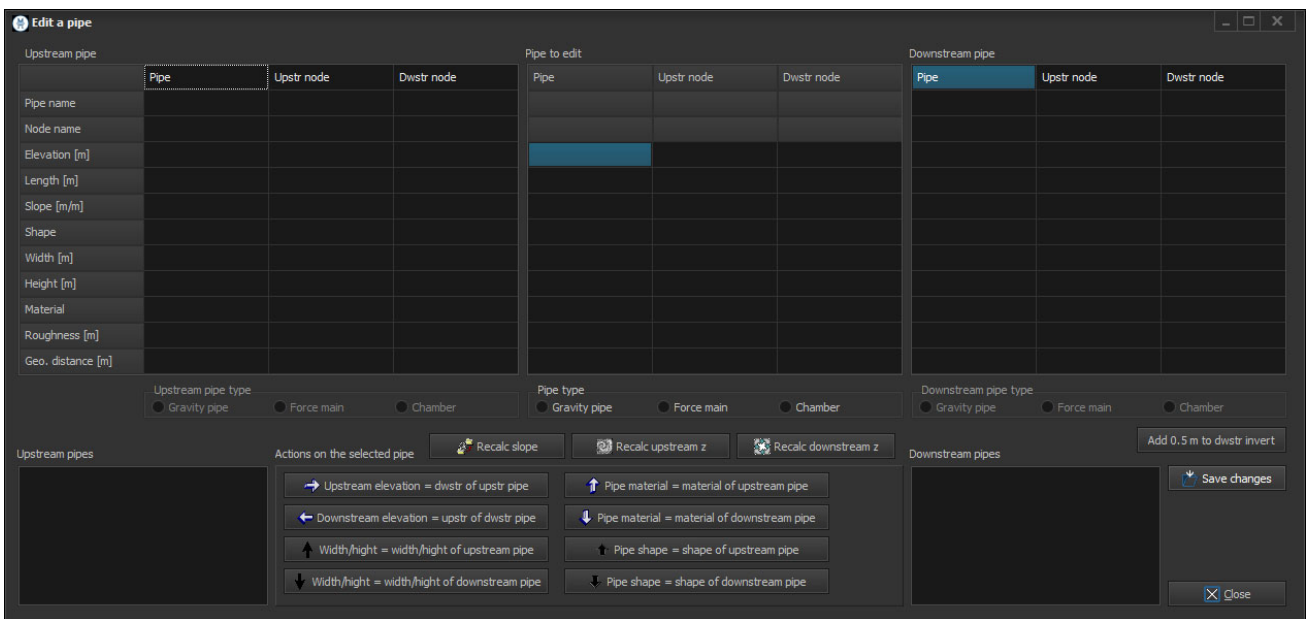
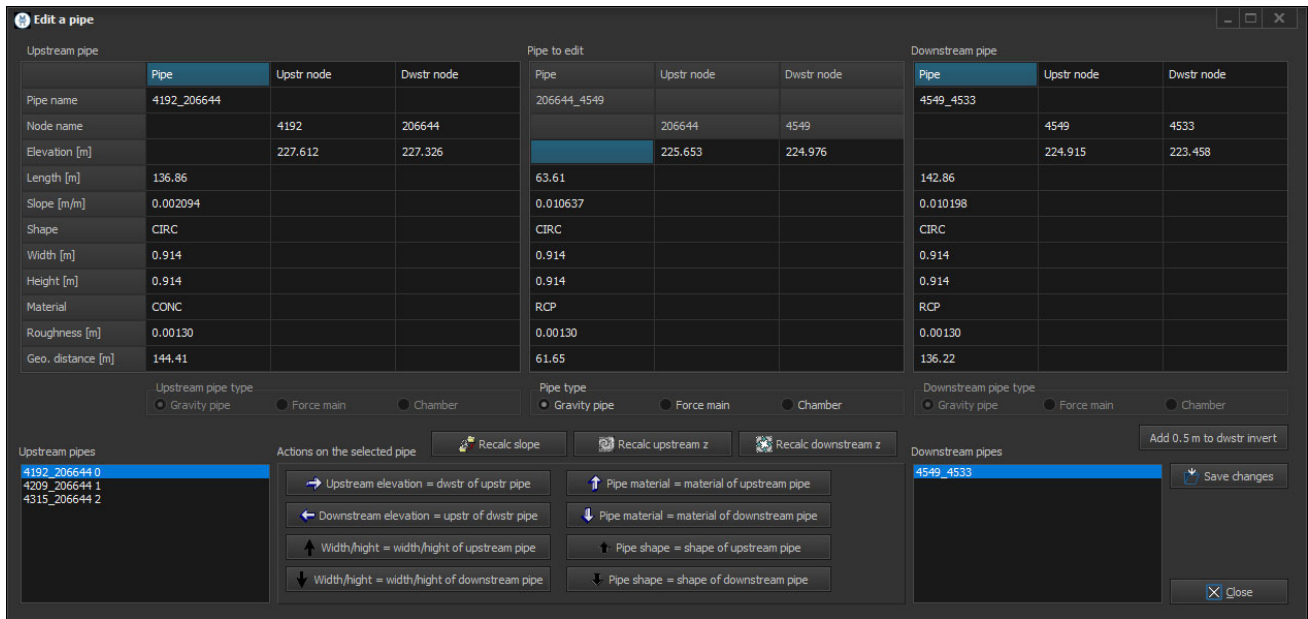


Figure 71. Edit a pipe form before populating it



Upstream pipe				Pipe to edit			Downstream pipe		
Pipe	Upstr node	Dwstr node		Pipe	Upstr node	Dwstr node	Pipe	Upstr node	Dwstr node
Pipe name	4192_206644			206644_4549	206644	4549	4549_4533	4549	4533
Node name		4192	206644						
Elevation [m]		227.612	227.326		225.653	224.976		224.915	223.458
Length [m]	136.86			63.61			142.86		
Slope [m/m]	0.002094			0.010637			0.010198		
Shape	CIRC			CIRC			CIRC		
Width [m]	0.914			0.914			0.914		
Height [m]	0.914			0.914			0.914		
Material	CONC			RCP			RCP		
Roughness [m]	0.00130			0.00130			0.00130		
Geo. distance [m]	144.41			61.65			136.22		

Upstream pipe type:  Gravity pipe  Force main  Chamber

Pipe type:  Gravity pipe  Force main  Chamber

Downstream pipe type:  Gravity pipe  Force main  Chamber

Upstream pipes: 4192\_206644 0, 4209\_206644 1, 4319\_206644 2

Downstream pipes: 4549\_4533

Actions on the selected pipe: Recalc slope, Recalc upstream z, Recalc downstream z

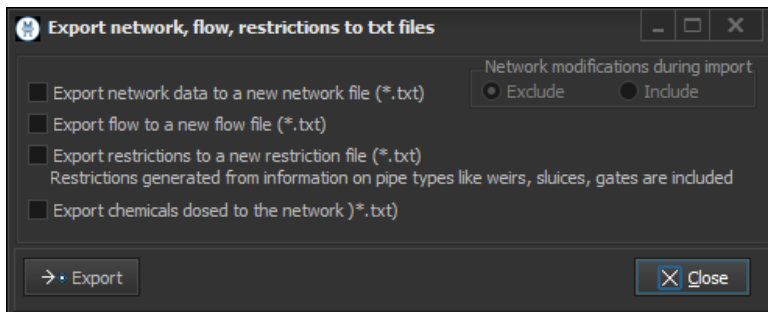
Buttons: Upstream elevation = dwstr of upstr pipe, Downstream elevation = upstr of dwstr pipe, Width/height = width/height of upstream pipe, Width/height = width/height of downstream pipe, Pipe material = material of upstream pipe, Pipe material = material of downstream pipe, Pipe shape = shape of upstream pipe, Pipe shape = shape of downstream pipe

Additional options: Add 0.5 m to dwstr invert, Save changes, Close

Figure 72. Populated Edit a pipe form

## 5.9 Export network, flows, restrictions, chemicals

Upon changing the network, its flows, restrictions and chemical dosing, the data must be exported to the text file format used by Mega-WATS (Figure 73).



**Export network, flow, restrictions to txt files**

Network modifications during import:  Exclude  Include

Export network data to a new network file (\*.txt)

Export flow to a new flow file (\*.txt)

Export restrictions to a new restriction file (\*.txt)  
Restrictions generated from information on pipe types like weirs, sluices, gates are included

Export chemicals dosed to the network (\*.txt)

Buttons: Export, Close

Figure 73. Form to export network, flows, restrictions, chemicals

### 5.9.1 Export network

After modifying the network, the new network data file can be exported into the same format as the original network file (section 4.2.1). There is a need for this after the automatic filling in of information when loading an incomplete data file (Section 5.2). In this case one can choose also to export a list of all the modifications done automatically. The network furthermore needs to be exported after having been modified it as describe in section 5.8.

### 5.9.2 Export flow

In some cases, flow file exports from hydrodynamic models contain a lot of repetitive information, for example the same node receiving many small inflows, and often zero-inflows. Reading the flow file into Mega-WATS simply adds all those flows to a node into one value (section 4.2.2). However, if the extent of



this is large, the reading of the flow file is comparatively slow. To speed up the process, it makes sense to export a consolidated flow file where there is only one flow per node.

Exporting flow is needed when the flow has been modified upstream of some location(s) in the network file (section 5.10).

### 5.9.3 Export restrictions

Mega-WATS can automatically set flow restrictions, or this can be done manually (section 4.2.3.1). Upon doing this, a restriction file must be exported. It holds all automatically set flow diversions as well as earlier loaded flow restrictions and diversions.

### 5.9.4 Export chemicals

Chemicals can be dosed through the GUI (section 10.2). Upon doing this, a dosing file must be exported. It holds all new dosing as well as earlier loaded dosing (section 4.2.5).

## 5.10 Modify flow in the network

The flow upstream of a selected pipe can be changed in the *Tools -> Modify upstream flow* menu (Figure 3). The form in Figure 74 allows selecting a pipe and then modifying the flow to the upstream node of the selected pipe and all upstream nodes by a factor.

The pipe can be selected on the map, and the pipe name transferred by clicking the button *Select pipe for modification*. Alternatively, the name of the pipe can be typed or copied manually into the edit field. The *Show network to be modified* button highlights the selected section of the network. The factor by which all upstream input flow is modified is typed into the edit field *Factor by which flow is modified upstream of pipe*. Pressing the button *Modify and write flow file* will highlight the selected part of the network and allow choosing a name for the new flow file. The new flow file holds all data from the old flow file, but with the flow to the nodes of the selected pipes modified by the factor. The modification can be done for average flows and for diurnal flow variations.

The project must be rebuilt with the modified flow file for the changes to take effect.

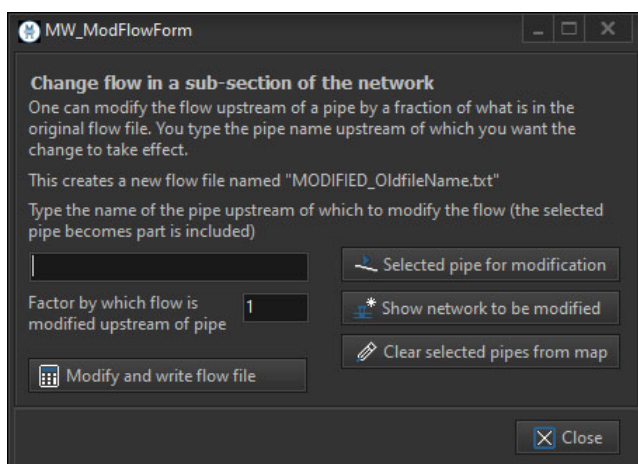


Figure 74. Modifying flow upstream of a pipe

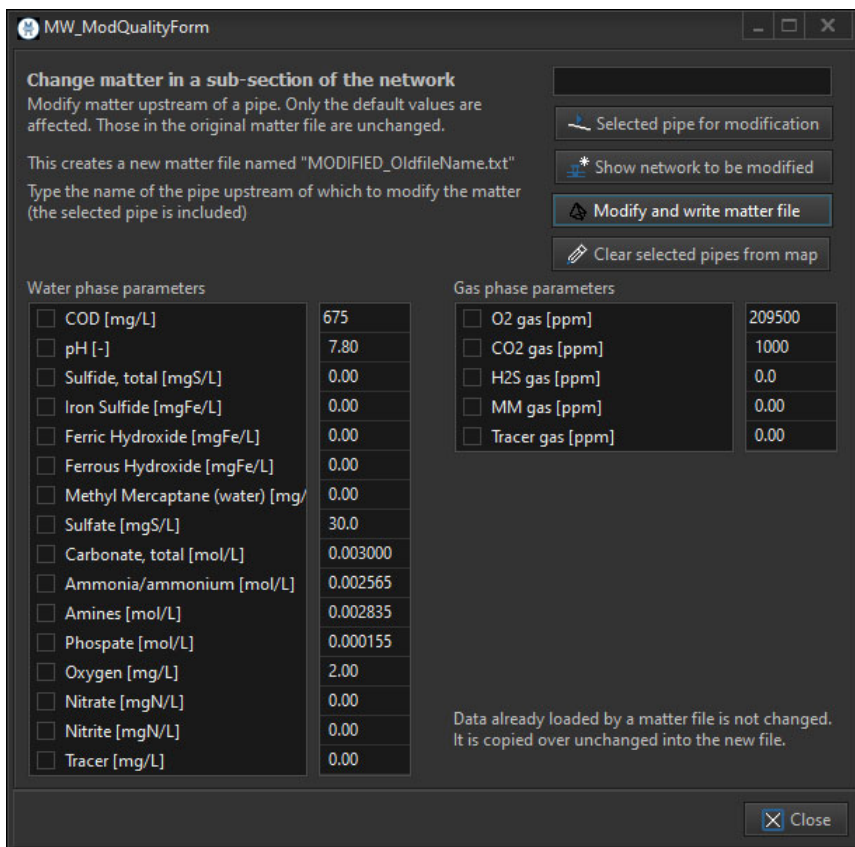
### 5.11 Modify water quality in the network

The flow upstream of a selected pipe can be changed in the *Tools -> Modify upstream matter* menu (Figure 3). The form in Figure 75 allows selecting a pipe and then modifying the matter of the flow entering the upstream node of the selected pipe and all upstream nodes.

The pipe can be selected on the map, and the pipe name transferred by clicking the button *Select pipe for modification*. Alternatively, the name of the pipe can be typed or copied manually into the edit field. The *Show network to be modified* button highlights the selected section of the network.

The matter contained in the flow to the upstream nodes is set to the values in the string grids (to the right of the parameters). One grid for parameters in the water, and one for parameters in the sewer air. The checkboxes left of the parameter names must also be checked for the action to take effect. Pressing the button *Modify and write matter file* will highlight the selected part of the network and allow choosing a name for the new matter file. The new matter file holds all data from the old matter file, but with the matter to the nodes of the selected pipes modified. If the old matter file holds an entry in the selected network, the value from the old matter file is preserved. The modification can be done for average flows and for diurnal flow variations.

The project must be rebuilt with the modified matter file for the changes to take effect.



**Change matter in a sub-section of the network**  
 Modify matter upstream of a pipe. Only the default values are affected. Those in the original matter file are unchanged.  
 This creates a new matter file named "MODIFIED\_OldfileName.txt"  
 Type the name of the pipe upstream of which to modify the matter (the selected pipe is included)

Selected pipe for modification  
 Show network to be modified  
 Modify and write matter file  
 Clear selected pipes from map

Water phase parameters		Gas phase parameters	
<input type="checkbox"/> COD [mg/L]	675	<input type="checkbox"/> O2 gas [ppm]	209500
<input type="checkbox"/> pH [-]	7.80	<input type="checkbox"/> CO2 gas [ppm]	1000
<input type="checkbox"/> Sulfide, total [mgS/L]	0.00	<input type="checkbox"/> H2S gas [ppm]	0.0
<input type="checkbox"/> Iron Sulfide [mgFe/L]	0.00	<input type="checkbox"/> MM gas [ppm]	0.00
<input type="checkbox"/> Ferric Hydroxide [mgFe/L]	0.00	<input type="checkbox"/> Tracer gas [ppm]	0.00
<input type="checkbox"/> Ferrous Hydroxide [mgFe/L]	0.00		
<input type="checkbox"/> Methyl Mercaptane (water) [mg/	0.00		
<input type="checkbox"/> Sulfate [mgS/L]	30.0		
<input type="checkbox"/> Carbonate, total [mol/L]	0.003000		
<input type="checkbox"/> Ammonia/ammonium [mol/L]	0.002565		
<input type="checkbox"/> Amines [mol/L]	0.002835		
<input type="checkbox"/> Phosphate [mol/L]	0.000155		
<input type="checkbox"/> Oxygen [mg/L]	2.00		
<input type="checkbox"/> Nitrate [mgN/L]	0.00		
<input type="checkbox"/> Nitrite [mgN/L]	0.00		
<input type="checkbox"/> Tracer [mg/L]	0.00		

Data already loaded by a matter file is not changed. It is copied over unchanged into the new file.

Close

Figure 75. Modifying matter upstream of a pipe

### 5.12 Extract network upstream and downstream of a pipe

Part of the network can be extracted upstream and downstream of a pipe (Figure 76). A total of 6 files are created: 3 for the upstream section (network, flow, matter) and 3 for the downstream section (network, flow, matter). Either type the name of the pipe from where to separate networks or click it on the map. Then click the *Select Pipe* button (the selected pipe becomes part of the upstream network).

The extracted networks (upstream and downstream) can now be loaded as new projects.

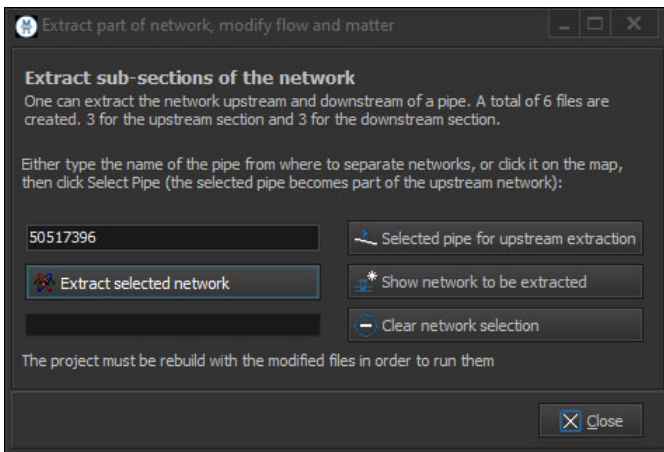


Figure 76. Extracting the network upstream of a pipe

### 5.13 Truncate a network

A network can be truncated by snipping a sub-network from it and simulating it as a stand-alone network. The truncating creates a new network file holding the snipped part, a flow file which holds the flow at the truncation boundary, and a matter file which holds the wastewater and air composition at the boundary. The latter two files contain the result of the model simulation at the boundary (all inflows to the truncated network). Running the truncated network will result in the same output as if the full network had been run. The benefit is to save time when doing detailed calculations of a sub-catchment in cases where simulation time is long. For example, when running diurnal simulations of large networks.

Go to the *Debug* page (Figure 4) and press the *Truncate network* button, and the truncation form is shown (Figure 77).

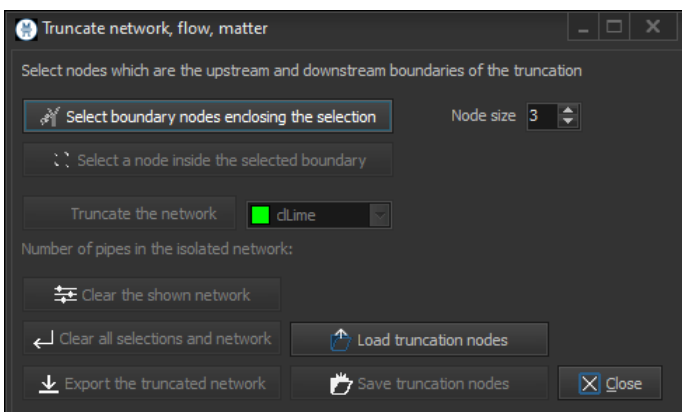


Figure 77. Truncating a network



Finally, the creation of the selection as a stand-alone network is done by the *Export the truncated network* button. If the model has been run with flow variation, the truncated network holds these flow and matter variations.

## 6 Visualizing model output on the GUI

Most of the model output of Mega-WATS is only a few clicks away. While this makes the graphical user interface (GUI) somewhat crowded, it also means that many things can be visualized rapidly.

The graphics of the GUI holds a map of the network layout (Figure 80) as well as plot-view graphics of every parametric value (Figure 81). The pages are available by clicking the *Flow and quality* page header and the *Network layout page* header, respectively.

To the left of the graphics is a list of all pipe names in the network. A pipe can be accessed by either clicking it on the map or by clicking its name in the list. If the list has focus (i.e., if a pipe has been clicked), one can also type the pipe name.

Below the list is a box holding various information on the selected pipe. In the example of Figure 80, a force main by the name of EYELSP\_TF21028201 was selected.

Below this are four pages with parameters that can be shown on the *Flow and quality* page (Figure 81). In the example, dissolved hydrogen sulfide in the wastewater was selected for viewing.

Below this there is a button for selecting chemical dosing (section 4.2.5).

To the right of the GUI map (Figure 80) are four pages giving access to view various parameters and aspects of the simulation, as well as some other facilities like debugging model errors.

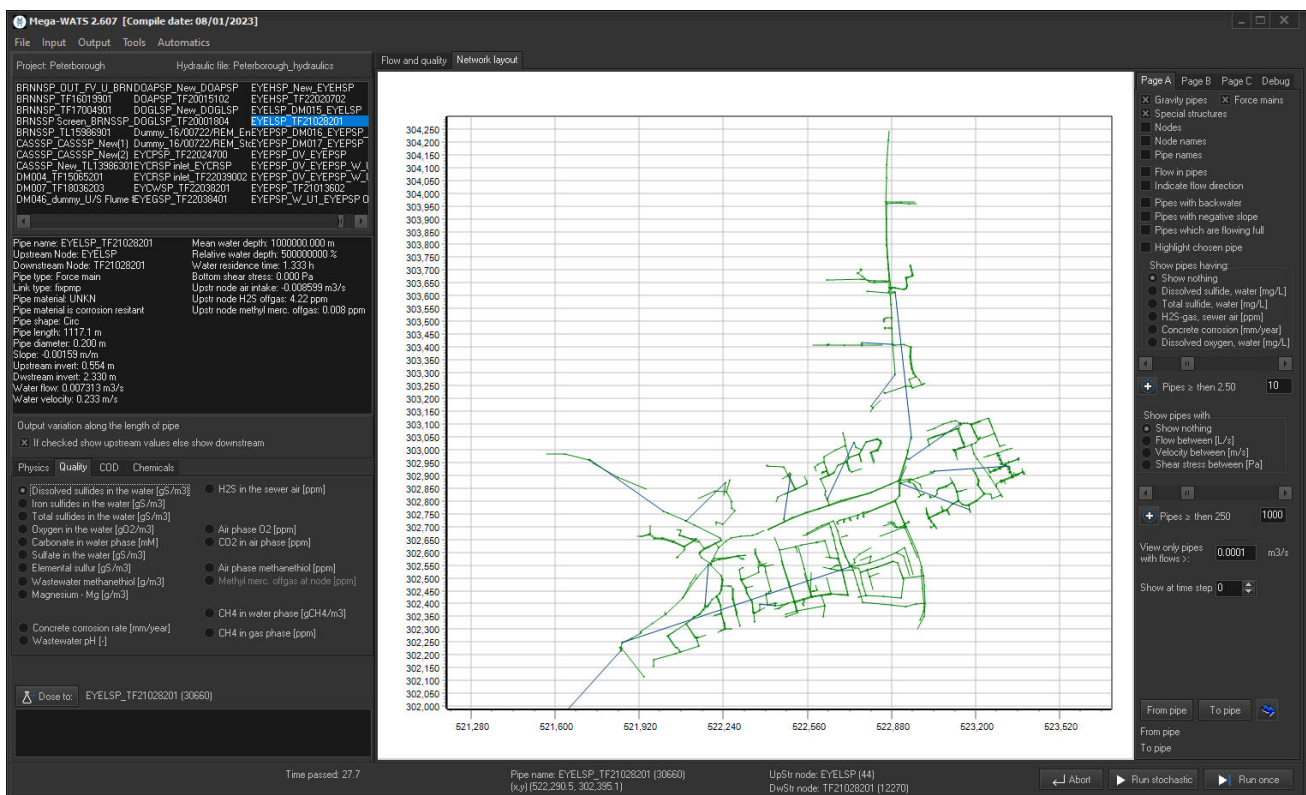


Figure 80. The map view of the graphical user interface (GUI)



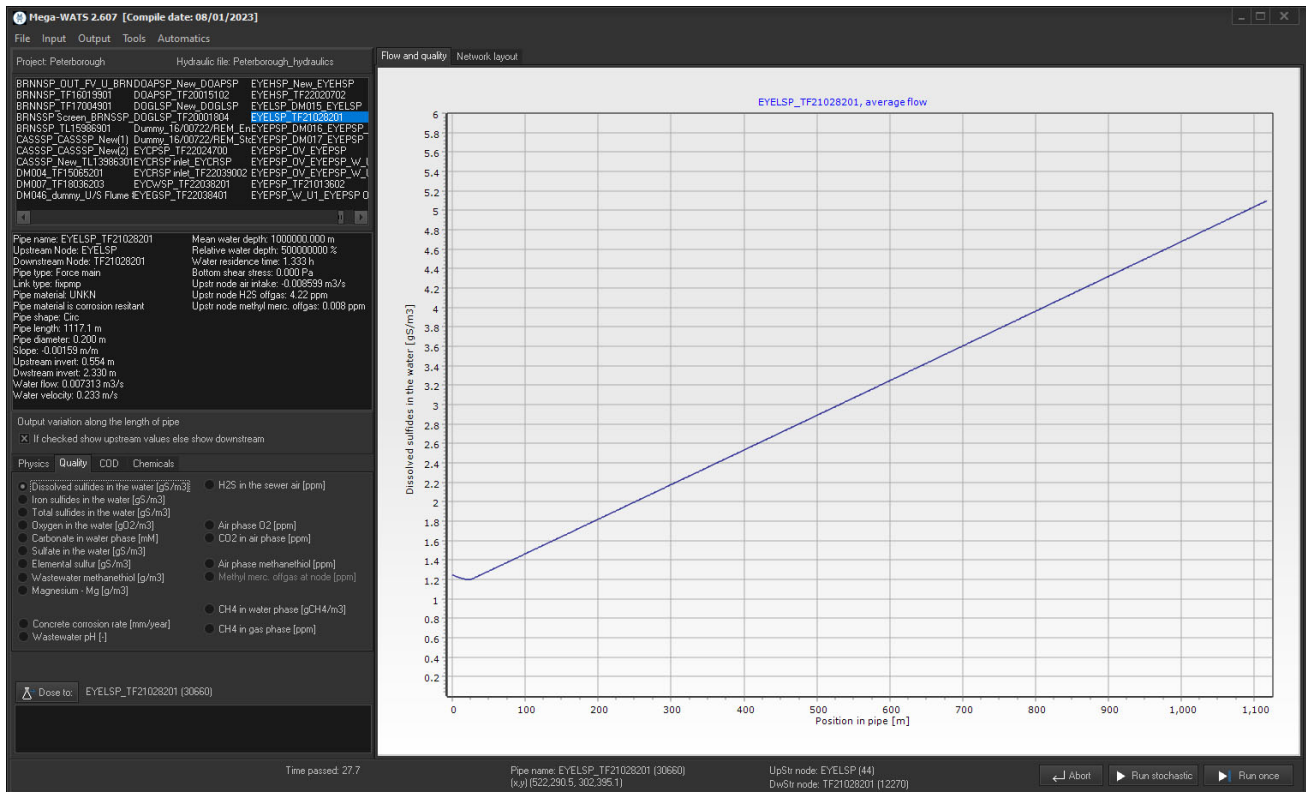


Figure 81. The parameter view of the graphical user interface (GUI)

## 6.1 Network layout

### 6.1.1 Showing pipes

Numerous options for showing the network layout are available. As default, Mega-WATS shows all gravity pipes, force mains, and special structures, where special structures cover chambers and treatment (section 4.2.1.5). The three types of pipes can be selected and un-selected on the top of *Page A* (Figure 4).

### 6.1.2 Showing nodes and names

Nodes can be shown by checking the *Nodes* checkbox below the *Gravity pipes*, *Force mains*, and *Special structures* checkboxes. They appear as small black circles. The names of nodes and pipes can be shown by checking the *Node names* and *Pipe names* checkboxes. Mega-WATS suppresses some of the names if the graphics gets too loaded with text, hence, to see all this info, one must zoom in on a part of the network (Figure 82).

### 6.1.3 Showing flow in pipes

One can also show the flow in the pipes by checking the *Flow in pipes* checkbox, however, then one must turn off the pipe name, as the two texts are placed at the same location.



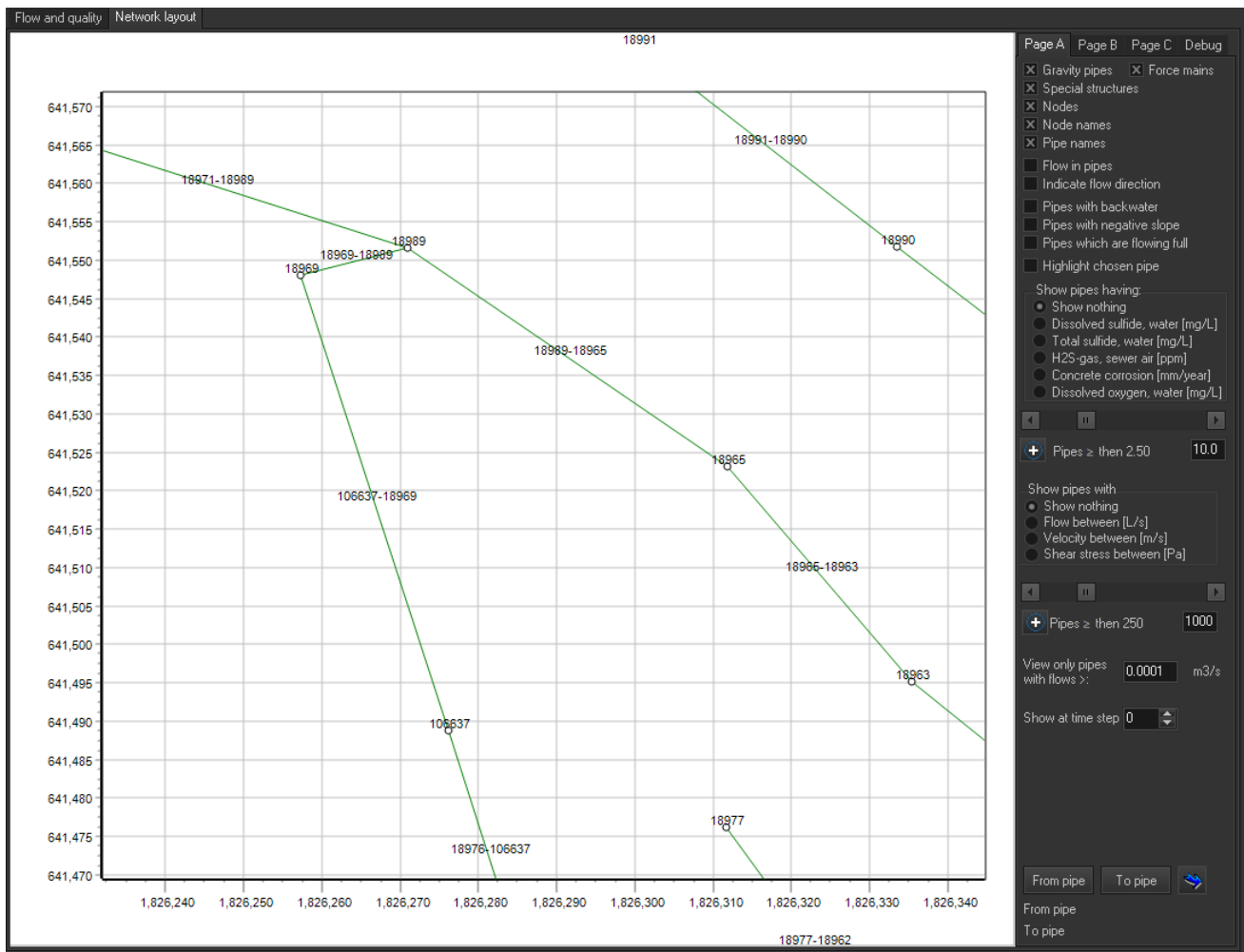


Figure 82. Showing pipes, nodes, node names, and pipe names

#### 6.1.4 Showing the flow direction

It can be quite difficult to keep an overview of flow direction. Checking the *Indicate flow direction* checkbox on *Page A* helps creating this overview (Figure 83).

#### 6.1.5 Highlighting a selected pipe

It can be quite difficult to keep track of which pipe is selected. Checking the *Highlight chosen pipe* checkbox on *Page A* helps to identify it (Figure 83).

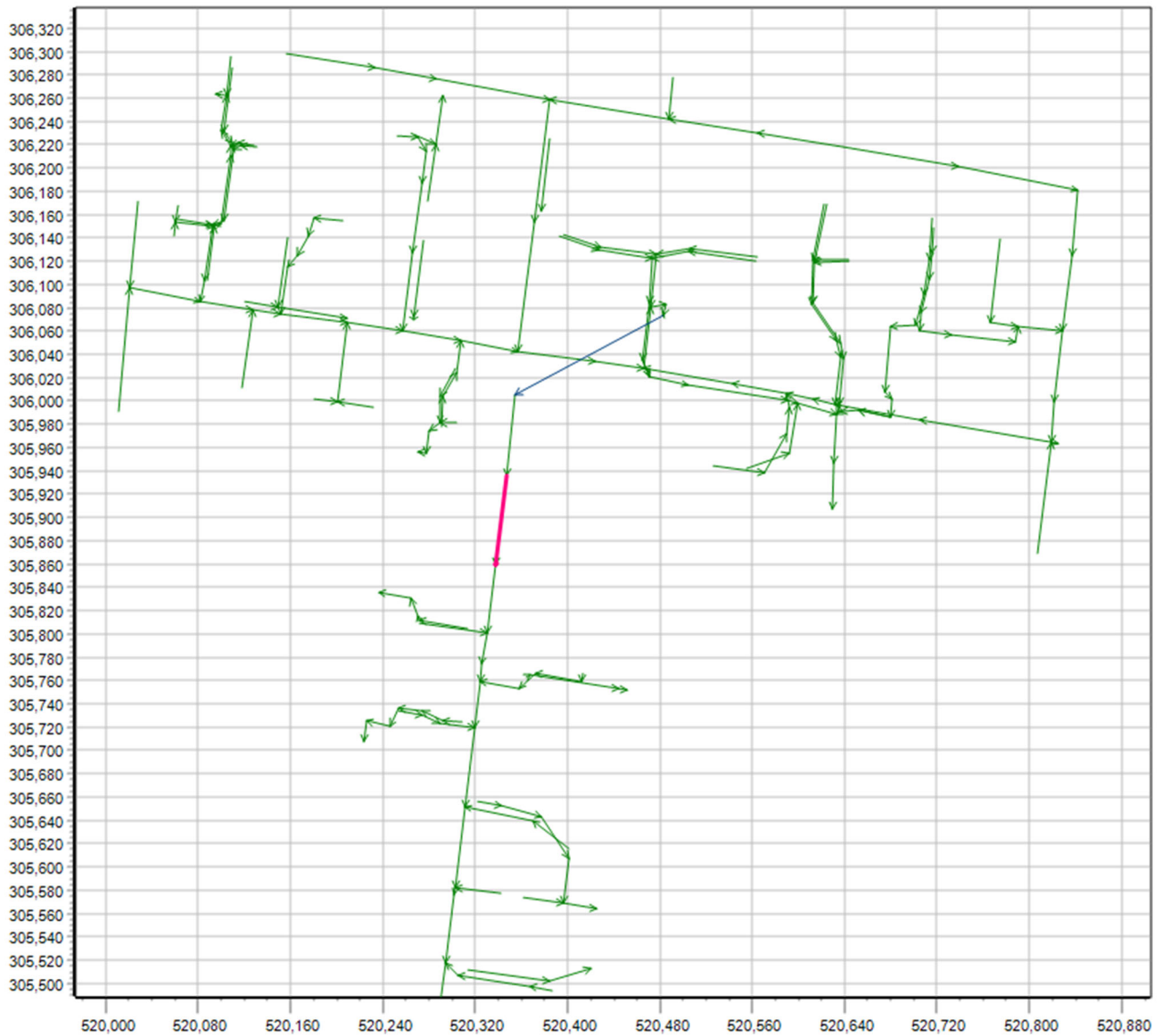


Figure 83. Direction of the flow in a network with one pipe selected and highlighted (pink)

## 6.2 The flow and quality parameters

Numerous flow and quality parameters can be shown using *Page A* (Figure 4).

### 6.2.1 Backwater in pipes

Mega-WATS calculates semi-stationary non-uniform flow (section 4.2.1.5.1), which means that backwater is calculated. If water for some reason stems up, or if it drops from one pipe to another, the flow in the pipe is no longer uniform, i.e., the water depth diverges from the normal depths established when gravitational drag and pipe wall friction balance out.

Figure 84 shows an example of such a case, where a small stretch of pipe has negative slope, creating backwater in that pipe as well as a small part of the upstream pipe.

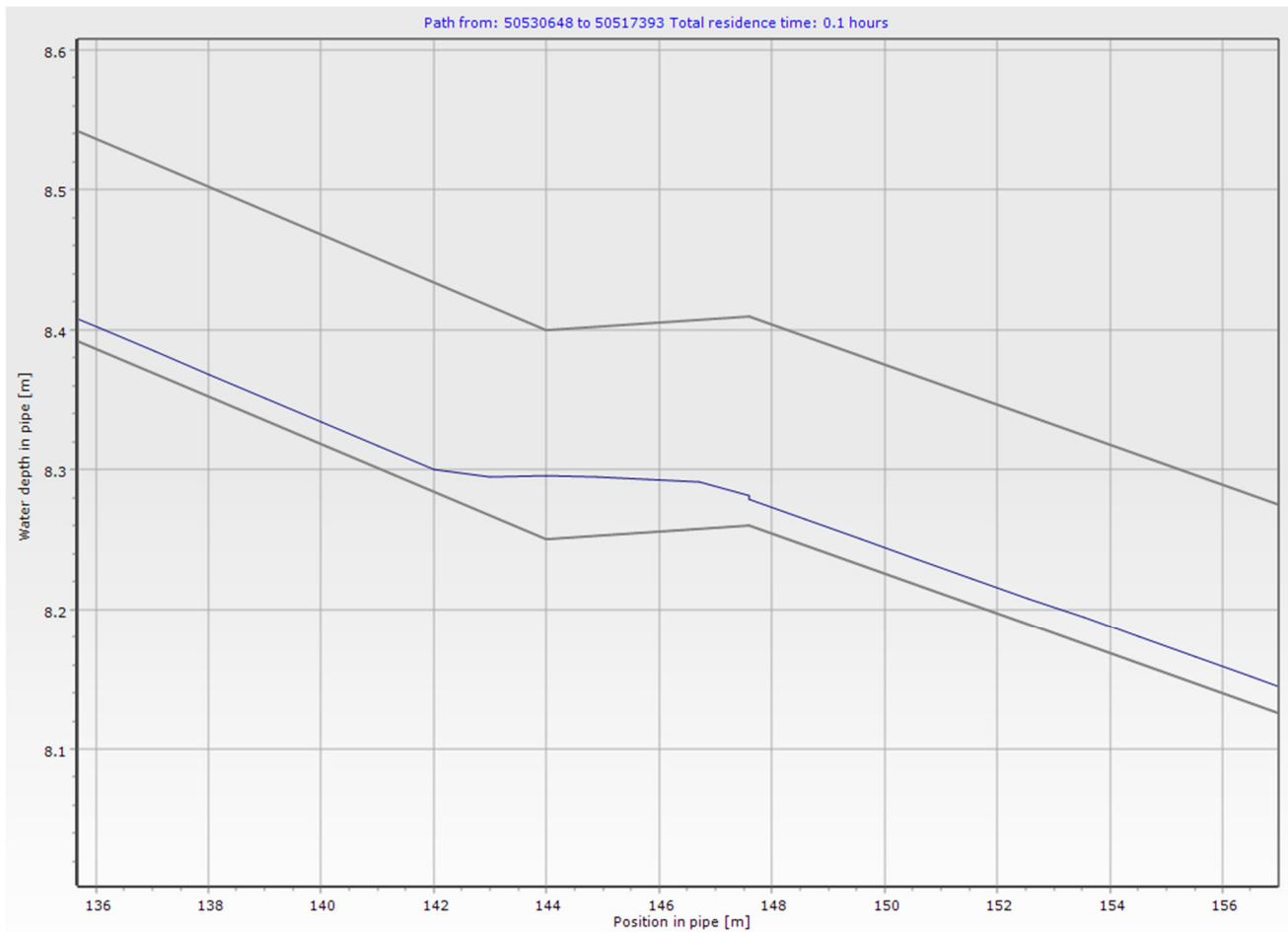


Figure 84. An example of backwater in a pipe

The places where a pipe experiences backwater can be shown on the network map by checking the *Pipes with backwater* checkbox on *Page A*. The pipes which have some part of them holding backwater are highlighted (Figure 85). In that figure, the pipe profile shown in Figure 84 is in the center of the map. The small pipe is marked, as is a longer upstream pipe. However, only the end of that part has backwater.

Which pipes get highlighted is governed by the setting in *Setup of units and more*, page *Showing on graph* (one can access the page from the main form menu: *Tools* → *Default network and flow settings*). The value in the form (1.5 as default) is the factor that normal depth is multiplied with to indicate 'serious backwater'. For example, if the normal depth in a pipe is 0.10 m, it will be included it some position in that pipe has a water depth  $\geq 1.5 \times 0.10 \text{ m} = 0.15 \text{ m}$ .

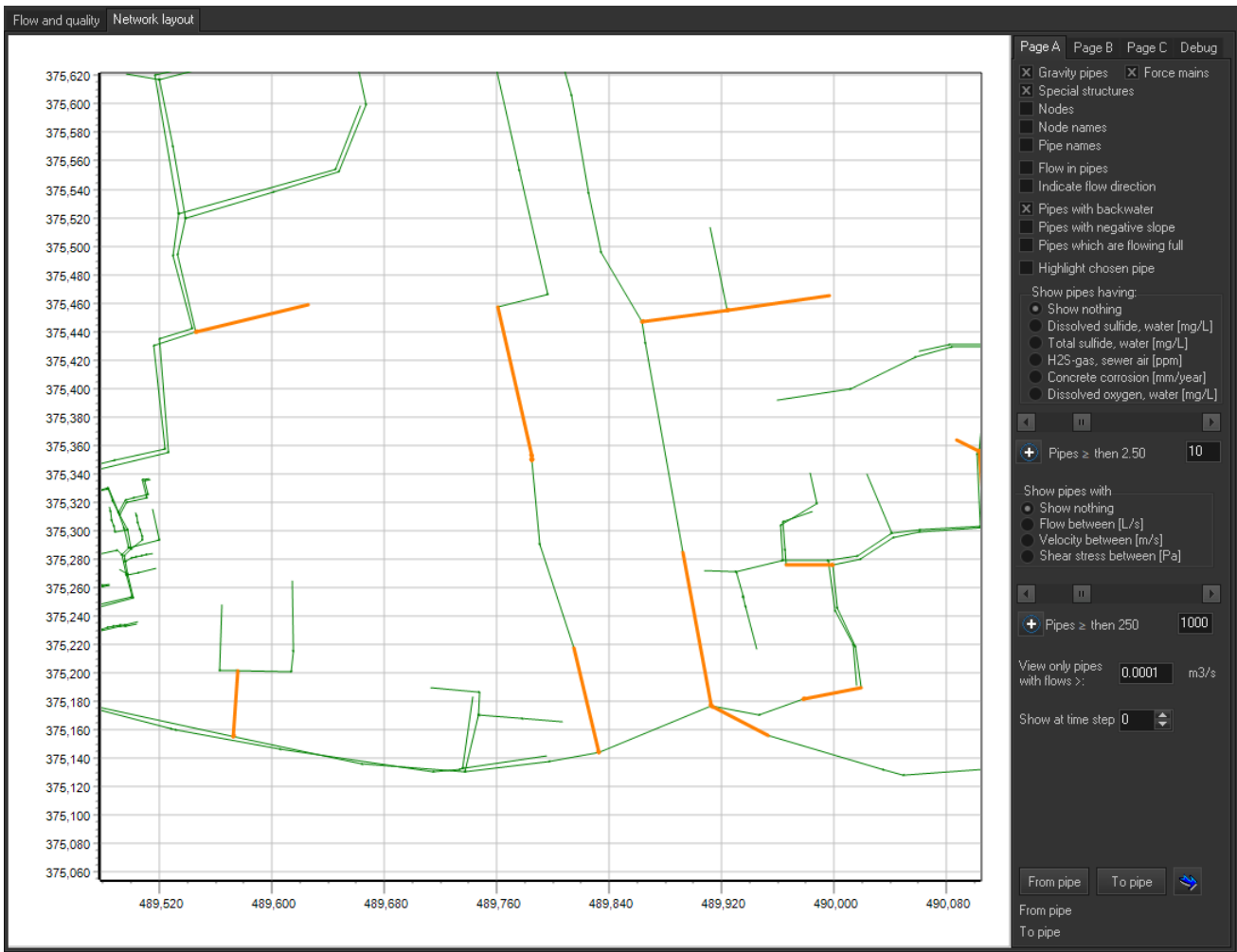


Figure 85. Pipes with backwater. The trigger value for when backwater is shown is set in the Setup of units and more form (Figure 86).

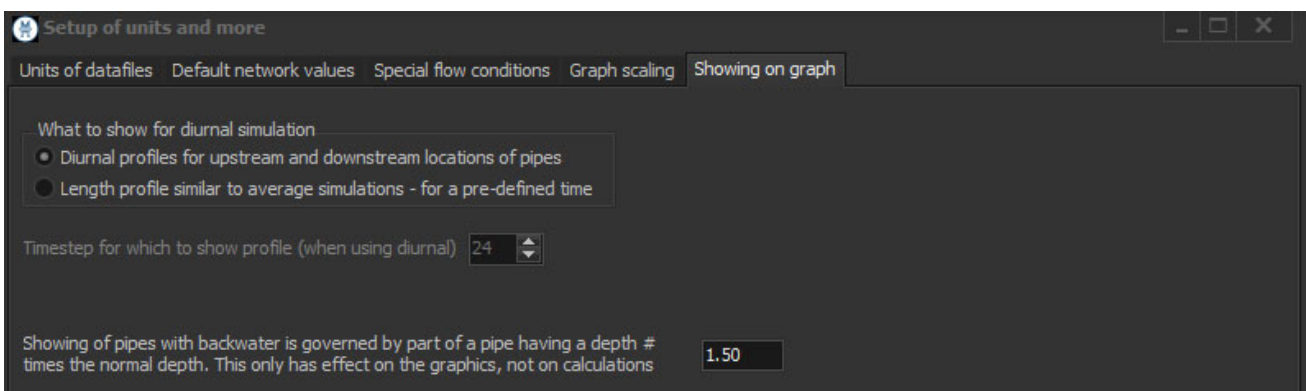


Figure 86. The trigger value for when backwater is shown, # times normal depth

### 6.2.2 Pipes with negative slope

Not all gravity pipes have positive slopes, and the GUI allows to show which have slopes below 0%. Check the *Pipes with negative slope* checkbox to visualize these.

### 6.2.3 Pipes which are flowing full

Some pipes flow full, either in one end, or in their full length. These pipes can be visualized by checking the *Pipes which are flowing full* checkbox.

### 6.2.4 Water and air quality in pipes

Pipes which have certain water and air qualities can be highlighted using the radio buttons under the menu *Show pipes having* on *Page A*. There are 5 parameters which can be visualized this way (Figure 87):

- Dissolved sulfide in the water (i.e., the  $\text{H}_2\text{S} + \text{HS}^- + \text{S}^{2-}$ )
- Total sulfide in the water (i.e., the sum of dissolved and metal bound sulfide)
- $\text{H}_2\text{S}$ -gas in the sewer air
- Concrete corrosion rates of moist surfaces
- Dissolved oxygen in the water

The trackbar below the radio buttons allow setting the actual value. The edit box at the lower right corner of Figure 87 allows setting the maximum value to show, i.e., the scaling covered by the track bar.

Pressing the + speed button to the left of 'Pipes ...' changes the  $\geq$  symbol to a  $\leq$  symbol, which means that instead of showing all pipes with a value above the chosen, all values below the chosen are shown.

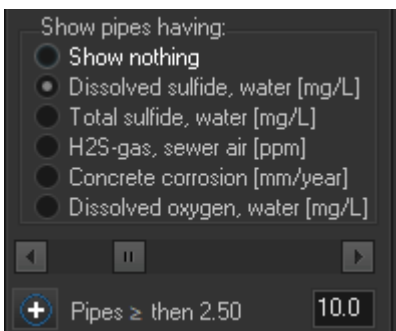


Figure 87. Visualizing pipes which have certain water and air qualities

The edit box *View only pipes with flows >*: is per default set to  $0.0001 \text{ m}^3/\text{s}$ . This is because simulations for very small flows are not that trustworthy. Hence small flows are cut off. This value can be set by the user.

Figure 88 shows one such example, where pipes with dissolved sulfide above  $1 \text{ mg/L}$  are highlighted.

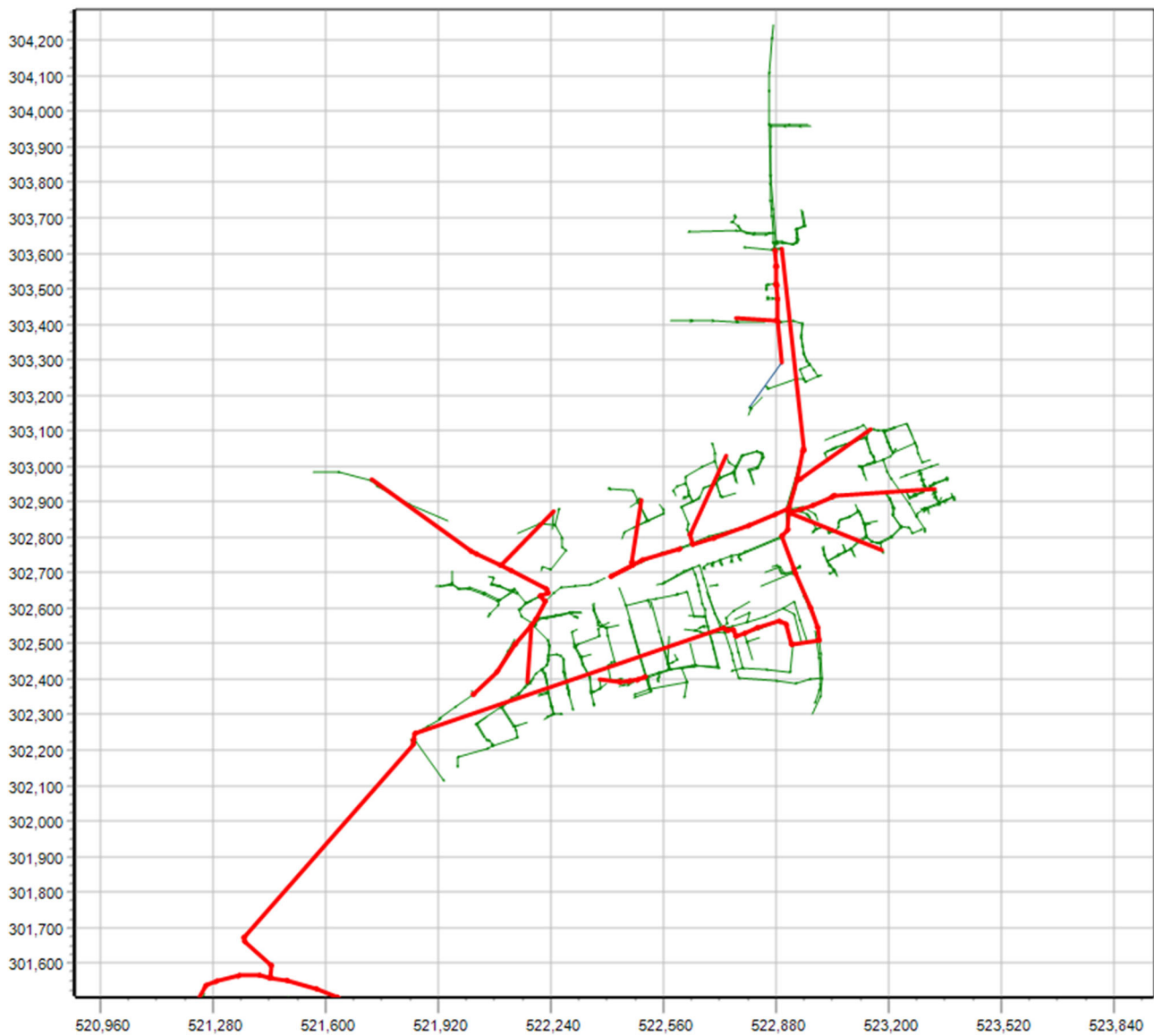


Figure 88. Pipes with dissolved sulfide above 1 mg/L

### 6.2.5 Flow parameters in pipes

Pipes which have certain flow characteristics can be highlighted using the radio buttons under the menu Show pipes with on Page A. There are 3 parameters which can be visualized this way (Figure 87):

- Flow
- Water velocity
- Shear stress

The setting of the values works as described for water and air quality in pipes in section 6.2.4.

### 6.3 The network map

While much of what can be shown is quite intuitive, there are some hidden aspects and some hints which can be helpful.

#### 6.3.1 Showing information on nodes

Checking the *Nodes* checkbox on *Page A* makes all nodes of the network visible. A hidden aspect here is that once the nodes are visible, they can be double-clicked to reveal details on that node (Figure 89).

The upper three boxes show information on the node, in this case a node called TF22029902. The number given (12694) refers to a Mega-WATS internal numbering of the node, which is also visible at the button of the main form (UpStr Node; DwStr node).

This node has no total volume, no water volume, and no air volume. This is the default of Mega-WATS. If a node is to be simulated holding air or water, for example if it is a wet well, it must be defined in the model setup applying a dedicated node file (section 4.2.8). The example node receives some water (0.000065 m<sup>3</sup>/s) and some air (0.000038 m<sup>3</sup>/s). The water has been defined in the flow file (section 4.2.2) while the air intake either has been calculated by Mega-WATS, is a result of an air flow file, or as been calculated by Mega-Vent (section 13.1, 4.2.6, 0, respectively). Had the pipe been corrodible, the corrosion of the node would have been set equal to the highest corrosion of the upstream end of the downstream pipes.

Below these three boxes are the flow and quality of the pipes entering the nodes, and then the flow and quality of the pipes exiting it.

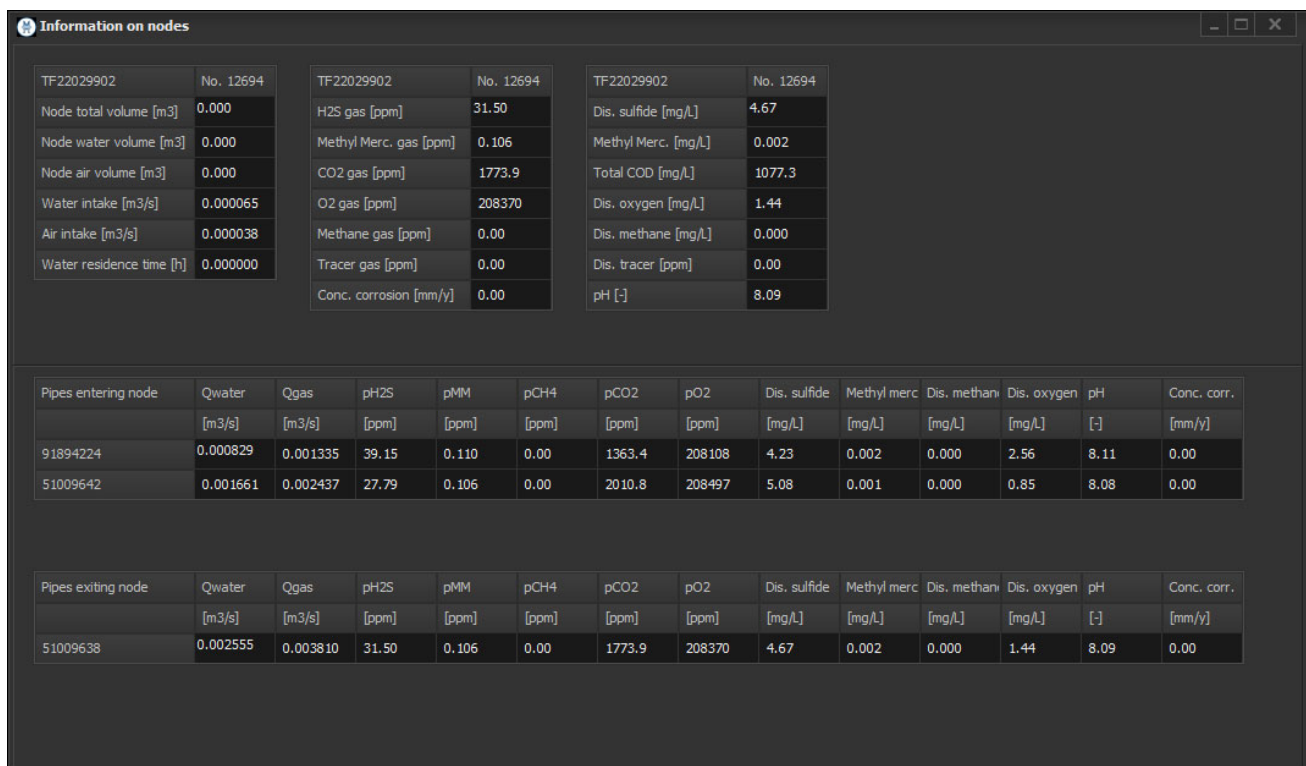


Figure 89. The Information on nodes form is shown when double-clicking a node



### 6.3.2 Show discharge points

On *Page B*, the first three checkboxes allow showing discharge points. The first shows the downstream terminus of hydraulically separated networks. There can be quite many of those, especially if the network includes separate foul sewers and storm sewers. Even though there is no flow, the endpoint of such a system is shown. Checking the box below eliminates all discharge points with no flow. Checking the third checkbox puts labels with flow and pipe names on the map.

### 6.3.3 Show nodes with inflow

On *Page B*, the panel with the three checkboxes Show nodes with inflow, Names, and Inflow allow showing the nodes which receive inflow according to the loaded flow file (section 4.2.2).

### 6.3.4 Show drops in the network

Drops are locations where one pipe enters a node at a higher elevation than the lowest pipe exiting it. These can be shown by checking the *Show drops in the network* checkbox of *Page B*. If only drops above a certain height shall be shown, this height is stated in the edit box below. The following checkbox, *Show height of step [m] n=0* shows the height of each drop on the map together with the drop. Once activated, the  $n=0$  changes to  $n=\#$ , where  $\#$  is the number of such drops in the network.

Figure 90 shows an example of visualizing drops. The orange arrow is the upstream point, with the arrowhead indicating the position of the drop. The number (1.28 m) is the drop height. This is a case where a side connection falls into an intercepting sewer line coming from the north and continuing towards the south-east.



Figure 90. Drops in a network

### 6.3.5 Show upwards steps

Upwards steps are often, but not always, errors in the network file (upwards steps can for example occur for syphons). In many network files these are quite common and must be removed during the debugging phase (section 5.7.2).

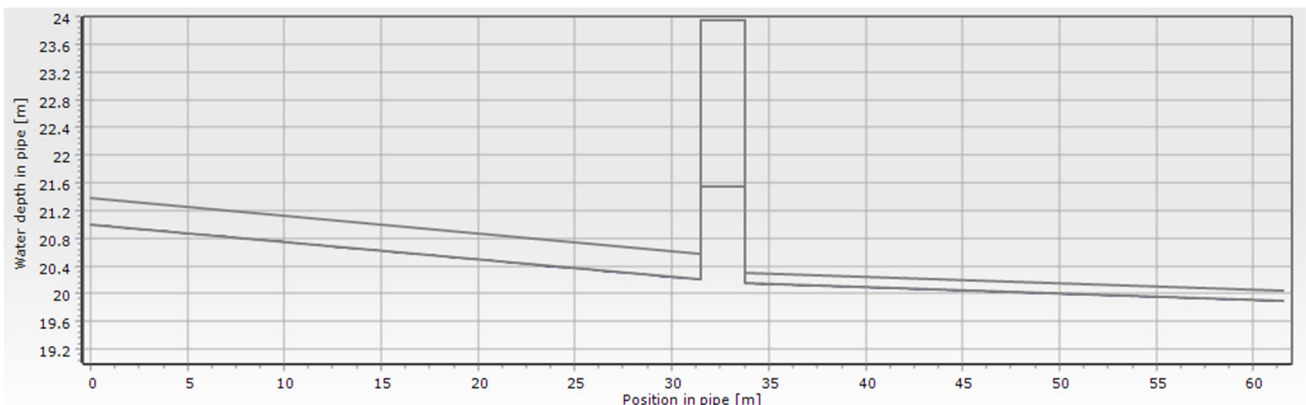


Figure 91. An upwards step in a network

### 6.3.6 Show sediments

The *Pipe sediments* > checkbox highlights pipes with sediments above the value given in the edit box to the right. Sediment depths must be loaded in the project setup (section 4.2.7). An example of a pipe stretch with sediments and the corresponding water depth is given in Figure 92.

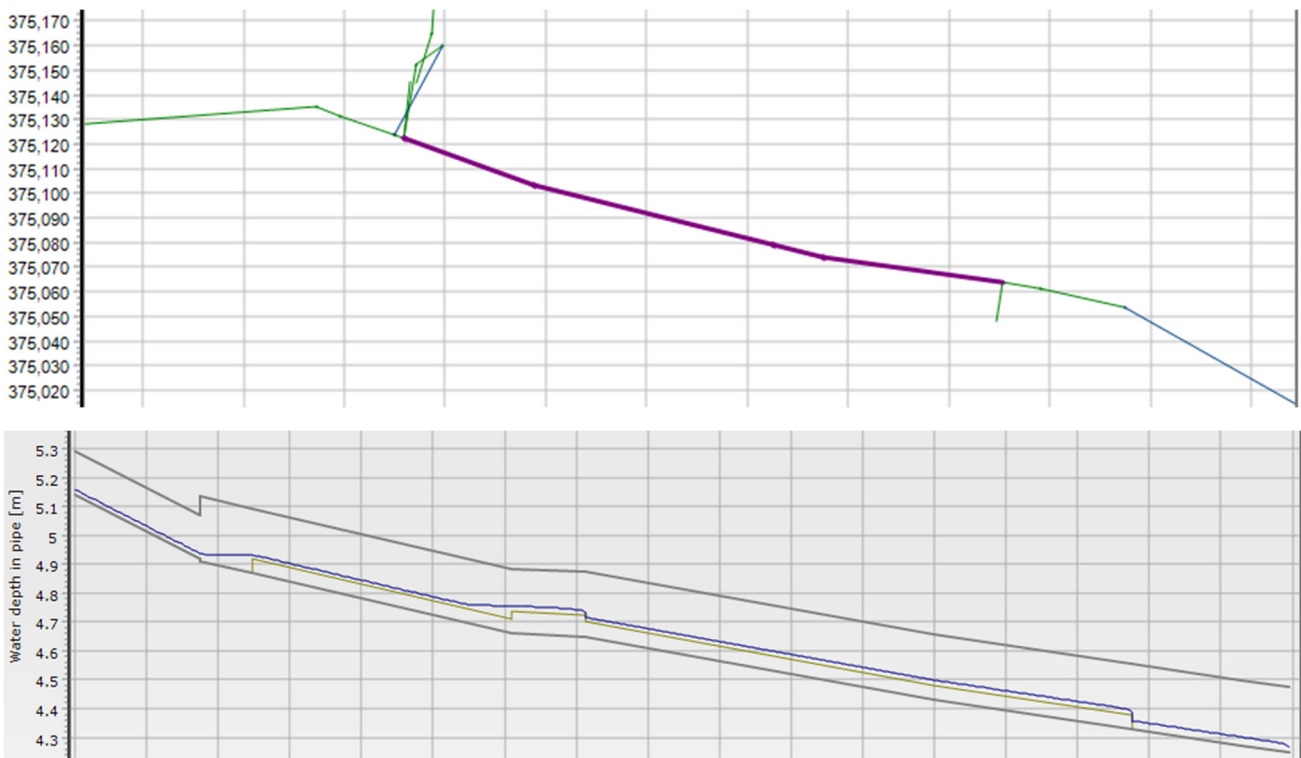


Figure 92. Sediments in a pipe

### 6.3.7 Show (x,y) callouts

Callouts based on map (x,y) coordinates must be loaded in the project setup (section 4.2.9). They are displayed by checking the *(x,y) callouts* checkbox. The callouts are displayed with the color loaded in the callout file. Checking the *Show (x,y) callout label* displays the label loaded from the file.

### 6.3.8 Show node callouts

Callouts based on map nodes must be loaded in the project setup (section 4.2.10). They are displayed by checking the *Node callouts* checkbox. The callouts are displayed with the color loaded in the callout file. Checking the *Show node callout label* displays the label loaded from the file.

### 6.3.9 Show gas equilibrium data

Gas equilibrium data must be loaded in the project setup (section 4.2.11). They are displayed by checking the *Gas equilibrium callouts* checkbox. The callouts are displayed with the color loaded in the callout file.

#### 6.3.10 Show chemical dosing locations

Locations where chemicals are dosed can have been loaded via the project setup (section 4.2.5) or during runtime (section 10.2). They are displayed by checking the *Chemical dosing locations* checkbox of *Page B*, using a preset color depending on the chemical. The name of the chemical can be displayed by checking the *Show type of chemical* checkbox.

#### 6.3.11 Show loaded nodes

Nodes loaded in the project setup (section 4.2.8) can be displayed by checking the *Show loaded nodes* checkbox or the *Show loaded nodes with water* checkbox of *Page B*. The color of the loaded nodes can be chosen by the color speed button to the right of the checkboxes.

#### 6.3.12 Show hydraulic jumps

Mega-WATS calculates hydraulic jumps as outlined in section 9.5.2. They are displayed by checking the *Show hydraulic jumps* checkbox of *Page B*. The color of the jumps can be chosen by the color speed button to the right of the checkbox.

#### 6.3.13 Show pump stations

Pump stations can be shown by checking the *Show pump stations* checkbox of *Page B*. The color of the pump stations can be chosen by the color speed button to the right of the checkbox.

#### 6.3.14 Show force main discharge nodes

Force main discharges can be shown by checking the *Show force main discharges* checkbox of *Page B*. The color of the pump stations can be chosen by the color speed button to the right of the checkbox.

#### 6.3.15 Show pipes upstream of a pipe

It can often be convenient to identify sub-catchments. This can be done using the *Mark pipes upstream of:* edit box and the buttons below it. Pipes are selected by selecting a pipe in the network (typically by clicking on the map) and then placing the cursor in the *Mark pipes upstream of:* edit box. This leads to the name being transferred to the edit box. If a pipe name does not exist, a warning is shown, and nothing is selected.

The color of the sub-catchment pipes can be chosen by the color speed button to the right of the *Mark upstream of* button. If the checkbox *Mark multiple upstream networks* is checked, then multiple selections using different colors can be made. Figure 93 shows an example of a major pump station (marked by light blue) and its two sub-catchments.



Figure 93. Two sub-catchments feeding a major pump station

### 6.3.16 Outgassing and air intake

The flowing water creates air flows and pressures which lead to air going in and out of the sewer. The air going out enters the urban atmosphere where it can cause odor problems. The amount of air taken in or pushed out of the sewer has either been calculated by Mega-WATS, is a result of an air flow file, or has been calculated by Mega-Vent (Sections 13.1, 4.2.6, 0, respectively). Whatever the approach, the radio buttons, check boxes, and edit boxes in the upper part of Page C allow this to be visualized. Checking one of the radio buttons, for example  $H_2S$  (34.08 g/mol) and the *Gas in and out at nodes* checkbox, results in red circles being displayed. If the checkbox *Air label (g/day)* is also checked, the flux of  $H_2S$ -gas in the unit g $H_2S$ /day is added as labels. The graphics will always show the circles (Figure 94).

However, due to restrictions in the software, labels are only shown when there are not too many of them. Hence, if one needs to see labels, it can be necessary to limit the area shown and the minimum and maximum flux. This is done by putting values into the *Min flux to show* edit box and the *Max flux to show*



edit boxes. Another reason to limit what is shown is that amounts of air and gases going in and out of sewers varies many orders of magnitude between nodes. The area of the circle is proportional to its corresponding value so some circles can hence totally overshadow the map view.

To manage the circles' appearance, their size scale can be adjusted by entering a value in the *Relative off-gas circle size*: edit box.

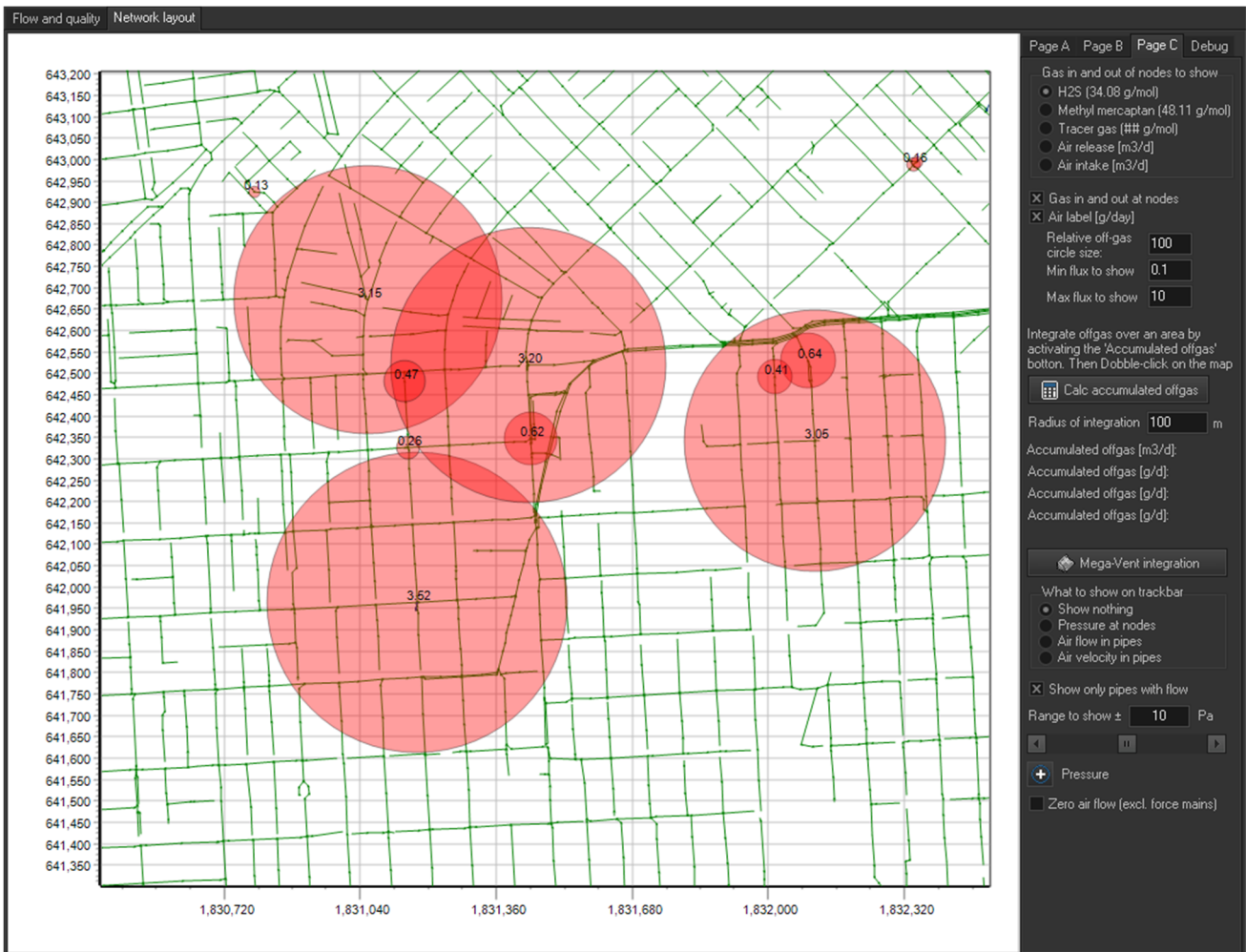


Figure 94. Flux of H<sub>2</sub>S-gas out of a sewer network

### 6.3.17 Integrating off-gas over an area

Mega-WATS shows the outgassing and air intake for each node. However, often nodes are close by, and outgassing should be added for several pipes. To facilitate this, Mega-WATS can combine all amounts of air and gases going in and out of sewers within a certain distance from a point. To do this, press the *Calc accumulated off-gas* button on the map where off-gasses are to be integrated into a single emission source. The distance from the point is set in the *Radius of integration* edit box.

Figure 95 shows one such example, where the total amount of air going out around this (quite large) pump station is 7,164,122 m<sup>3</sup>/d, holding 77.94 gH<sub>2</sub>S/d and 10.53 gMM/d (MM = Methyl Mercaptan). Such information can for example be utilized as input for odor dispersion modelling.

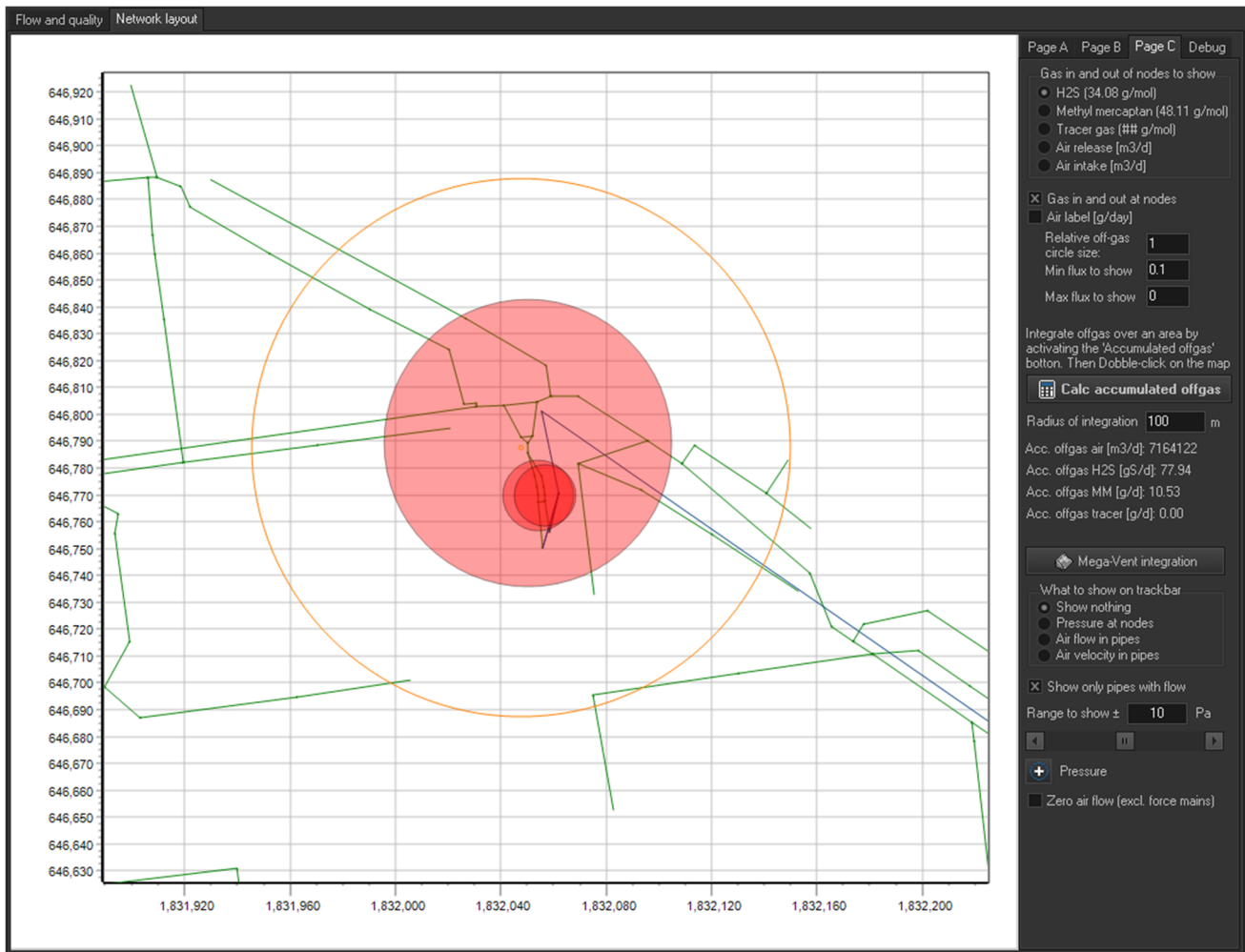


Figure 95. Integrating air and gases going in and out of sewers within a certain distance from a point

### 6.3.18 Show Mega-Vent integration

Mega-Vent is called using the *Mega-Vent integration* button of *Page C* (Section 3.1). If air flow was calculated by Mega-Vent, Mega-WATS holds air flow, air velocity, as well as air pressures from this calculation. If Mega-Vent was not run, all pressures are set to standard atmospheric pressures (101325 Pa).

The air flow and air velocity in pipes and the pressures at nodes can be visualized using the radio buttons below the *Mega-Vent integration* button of *Page C*.

## 7 Various information on the network

### 7.1 Show various characteristics

A variety of information can be shown on the network map (Figure 96 and Figure 97). The form for this is accessed from the *Debug* page, the button *Information on network*.

#### 7.1.1 Identify pipes with certain characteristics

The first checkbox in the top left corner defines which type of pipes are shown. The grid below allows choosing various characteristics to be shown on the map. The color of the markings can be changed by the



color speed button shown to the left of the button *Show pipes with the characteristics*. The selected pipes can be saved to a text file by the *Save pipes with the characteristics* button.

To the right of the grid, are all the pipe materials in the network listed. Selecting one or more materials and pressing the *Show materials* button will show pipes of the respective materials on the map. The color of the markings can be changed by the color speed button shown to the left of the button *Show pipes with the characteristics*.

In the lower left corner of the form, it is possible to highlight pipes which meet certain combinations of slope, water velocity, corrosion, sulfide, and H<sub>2</sub>S-gas.

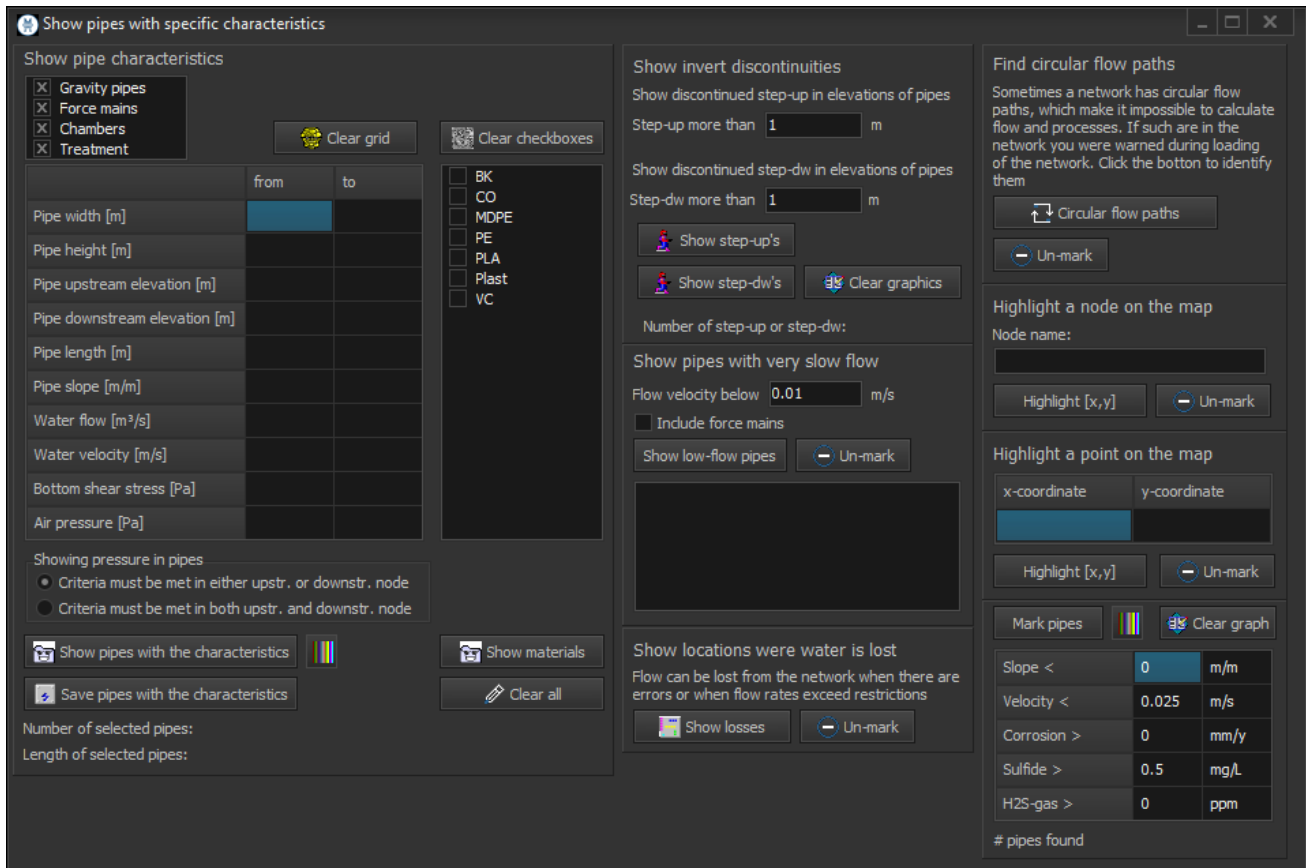


Figure 96. Information on network form when no pipe age has been loaded

### 7.1.2 Showing step-ups and step-downs

Step-ups and step-downs can be shown from this menu as well as from the *Page B*, choosing *Show drops in the network* and *Show upwards steps at nodes* (sections 6.3.4 and 6.3.5).

### 7.1.3 Identifying pipes with low flow velocities

Some pipes can have very low flow velocities, typically due to backwater. In the extreme, this can cause long simulation times, as the simulations are 'hanging' in a single pipe. These pipes can be identified by using the *Show low-flow pipes* button. Often these have no practical importance, and modifying the network to avoid them could be an option (section 5.3.5).

### 7.1.4 Highlighting nodes and x,y-coordinates

It can be difficult to find a specific node or coordinate on the map. To make this easier, the user can give a node name or x,y coordinates and then highlight them on the map (left part of the form).

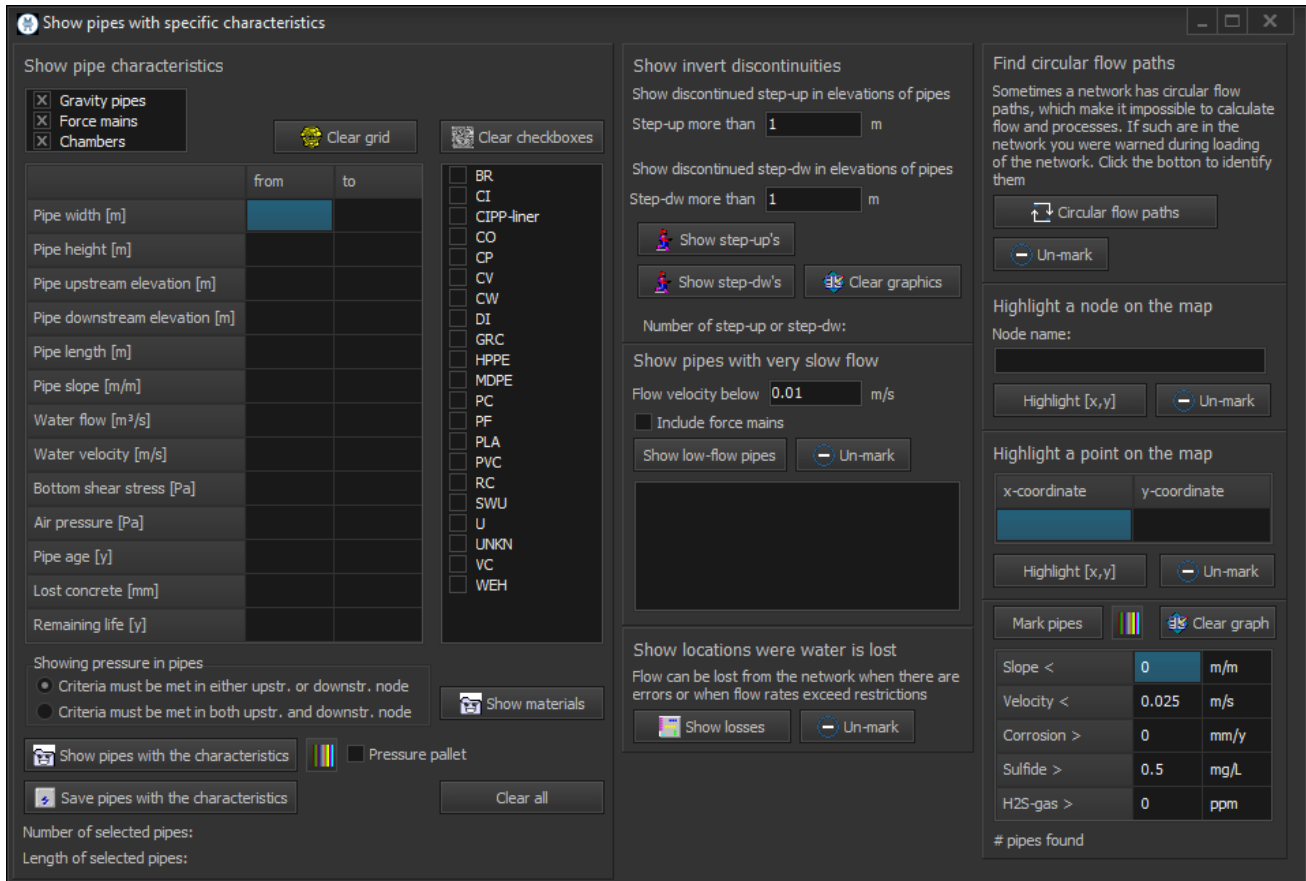


Figure 97. Information on network form if pipe age has been loaded

Nodes and pipes can furthermore be identified by using the field *Highlight a node or a pipe on the map* on the *Debug* page (Figure 4).

## 7.2 Remaining service life

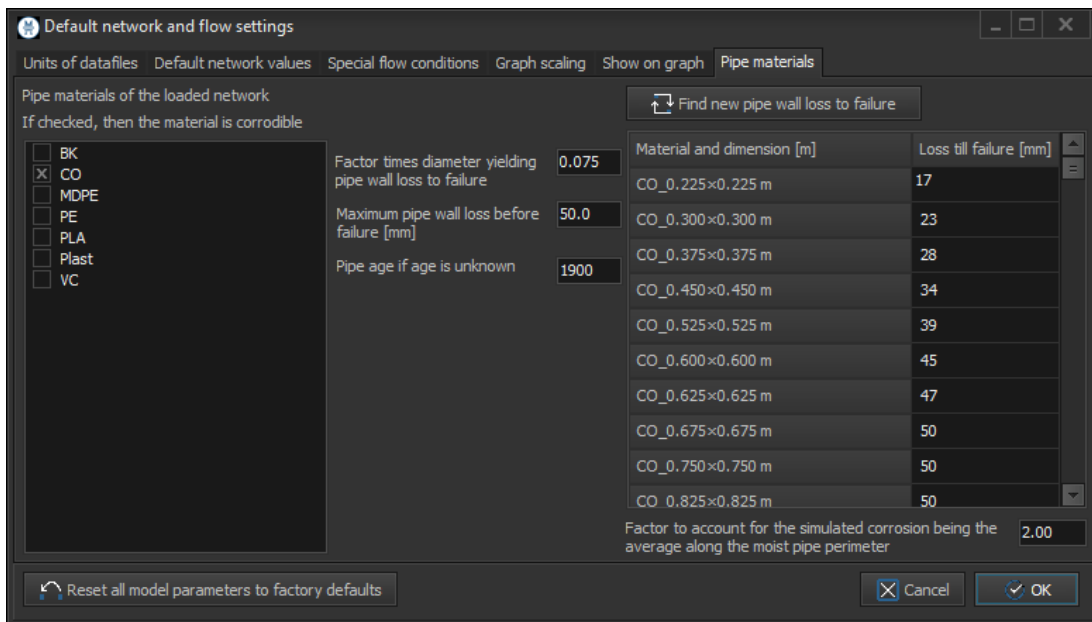
If the pipe age has been loaded (Section 4.2.1.12), the remaining service life can be predicted. Such prediction requires that the pipe material and its alkalinity is known; that the operational conditions from when it was put in place til now are known; and that a decision is made on how much pipe material can be lost before it is viewed as a failure.

Note that the simulated concrete corrosion is an average rate over the perimeter of the pipe (Section 9.4.13). Local corrosion rates will be higher or lower than the simulated value. It is for example common, that crown corrosion is more severe than corrosion on the vertical part of the pipe walls. The average corrosion rate should hence be multiplied by a factor to obtain the maximum corrosion rate, which will be the critical rate with respect to failure of a pipe. Albeit it remains uncertain how large such factor should be, it seems likely it is in the range of 1.5 – 2.5. This factor can be set in the *Set units and other parameters* form (Section 4.2.12 and Figure 98).

The alkalinity of the concrete is set as a global parameter as described in Section 9, or for each pipe as described in Section 4.2.1.13.

### 7.2.1 Setting the material loss till failure

The material loss till failure is set in the *Set units and other parameters* form (Section 4.2.12). The form is populated with all the corrodible pipes found in the loaded network (the grid on the left of Figure 98). Each distinct pipe diameter and material type is listed, and a default material loss till failure is calculate from the *Factor times diameter yielding pipe wall loss to failure* and the diameter. For example, if the factor is 0.075 and the diameter is 300 mm, then the material loss till failure is  $370 \times 0.075 = 28$  mm. if the diameters are large, this could potentially result in rather large material loss till failure, hence, a maximum is set, which can be seen as the cover layer of the rebar of reinforced concrete pipes.



Material and dimension [m]	Loss till failure [mm]
CO_0.225x0.225 m	17
CO_0.300x0.300 m	23
CO_0.375x0.375 m	28
CO_0.450x0.450 m	34
CO_0.525x0.525 m	39
CO_0.600x0.600 m	45
CO_0.625x0.625 m	47
CO_0.675x0.675 m	50
CO_0.750x0.750 m	50
CO_0.825x0.825 m	50

Figure 98. Pipe materials in the network and whether these are corrodible or not, as well as the allowed corrosion before end of service life

In case some pipes have no age, or the age is year zero, the default age given in *Pipe age if age is unknown* is used to predict remaining service life and total loss of concrete.

### 7.2.2 Showing accumulated material loss and time till failure on the GUI map

The accumulated loss over time as well as the remaining service life can be shown on the map of the GUI. The form for this is accessed from the *Debug* page, the button *Information on network* (Section 7.1.1 and Figure 97). In the grid to the left, state the interval of Lost concrete or Remaining life, the press Show pipes with the characteristics. Note that pipes were the age has not been loaded will be assumed having the age set as default (see above).

### 7.2.3 Showing accumulated material loss and time till failure on the GIS map

The accumulated loss over time as well as the remaining service life can be shown on a GIS map (Section 0). When pipe age has been loaded, the form looks slightly different from what is shown in Section 0, that is, three checkboxes are added, namely *Year placed*; *Lost Thickness*; and *Remaining life*. If *Remaining life* is chosen, two files will be created, one showing all the data for which pipe age was loaded, and one showing those data for which pipe age was assumed.

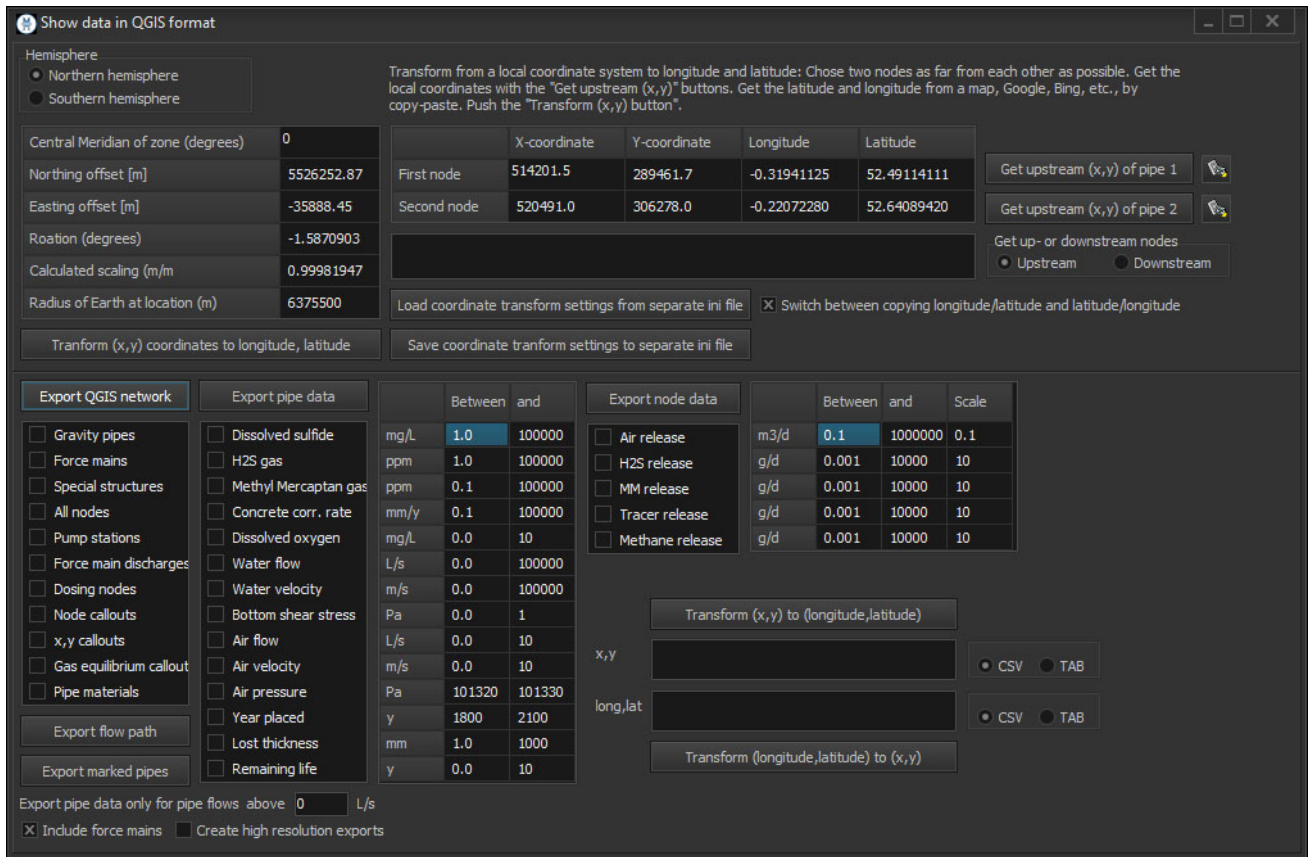


Figure 99. Export to QGIS form when pipe ages have been loaded

### 7.3 Accumulated corrosion

For simulation of diurnal variation, the accumulated corrosion over the duration of the simulation can be shown. This is done by selecting this option on the *Quality* tab (Figure 100). The view of *accumulated corrosion* is only shown for diurnal simulations, as this is the only case where accumulated corrosion can be calculated. It is furthermore necessary to set *What to show for diurnal simulation* to *Length profile similar to average simulations - for a pre-defined time* (section 4.2.12, Figure 41).

The corrosion is accumulated from the *Number of initial time steps ignored on graph when showing flow variation data*, which is as default set to 12 hours, and can be changed in the Default network and flow settings (section 4.2.12, Figure 40), to the end of the time series.

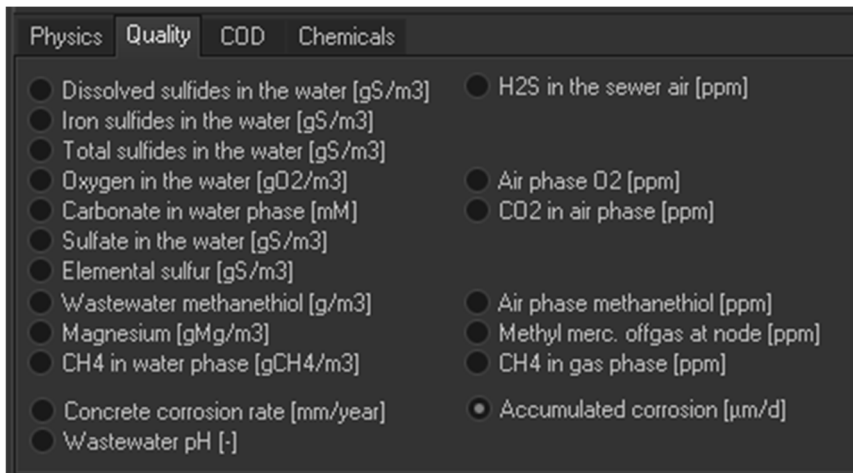


Figure 100. Choosing accumulated corrosion for diurnal flow simulations.

## 8 Running diurnal variations

In most cases, Mega-WATS is run for average conditions, but it can also run time-dependent variations, such as diurnal variations. Running diurnal variations is achieved by putting the diurnal patterns into the data files (section 4.2). The size of the time interval must be the same in all data files, as must the number of time steps. The *Run flow variation* check button must be checked before loading the flow file. After having loaded the flow file, other data files are loaded.

Simulations will take significantly longer than for running average conditions, as one simulation is run for each timestep. The output types are the same as for average conditions, but now the diurnal variation will be shown for each node instead of the changes along a flow path (Figure 101, Figure 102).

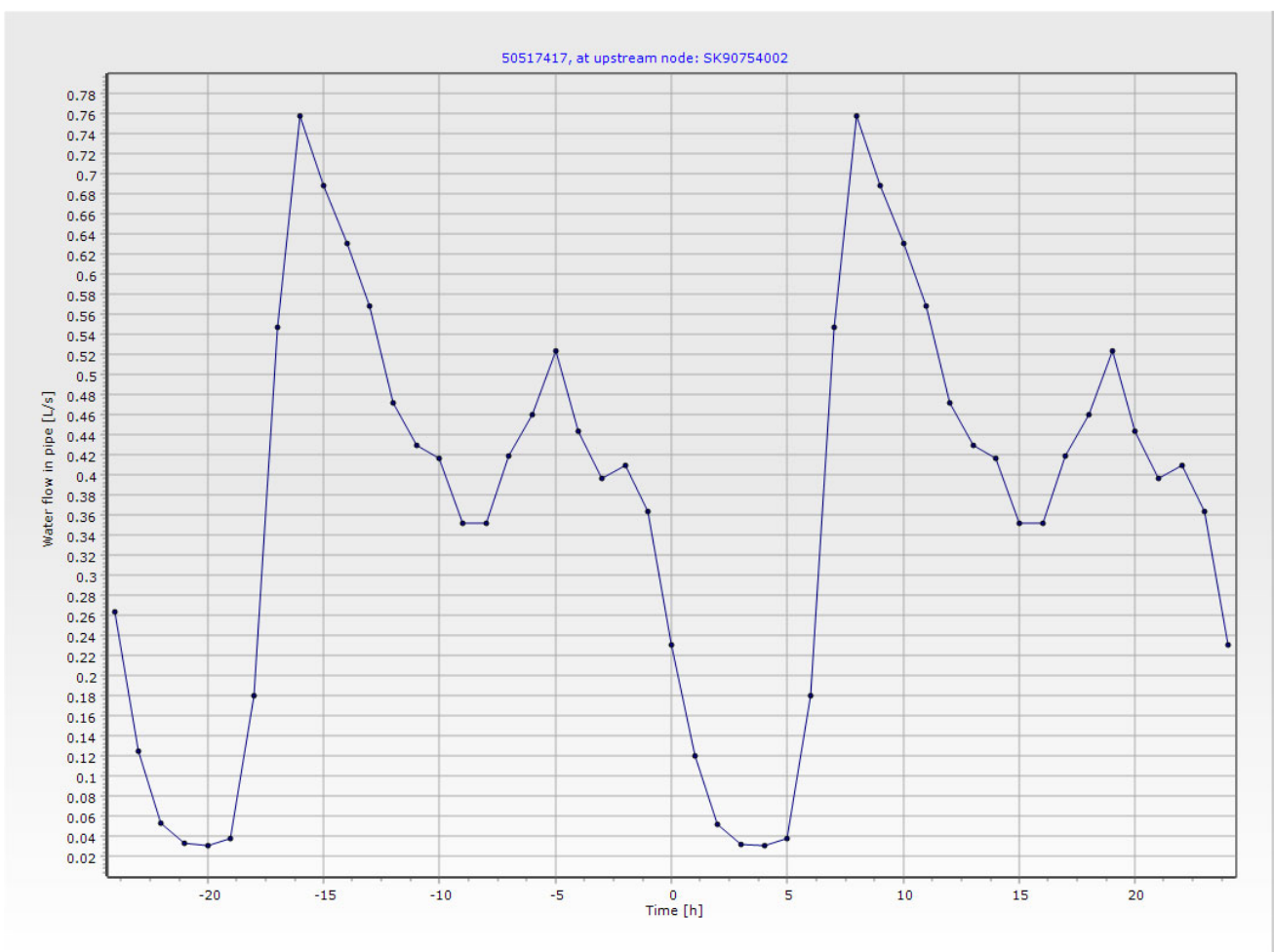


Figure 101. A diurnal simulation showing the simulated flow pattern

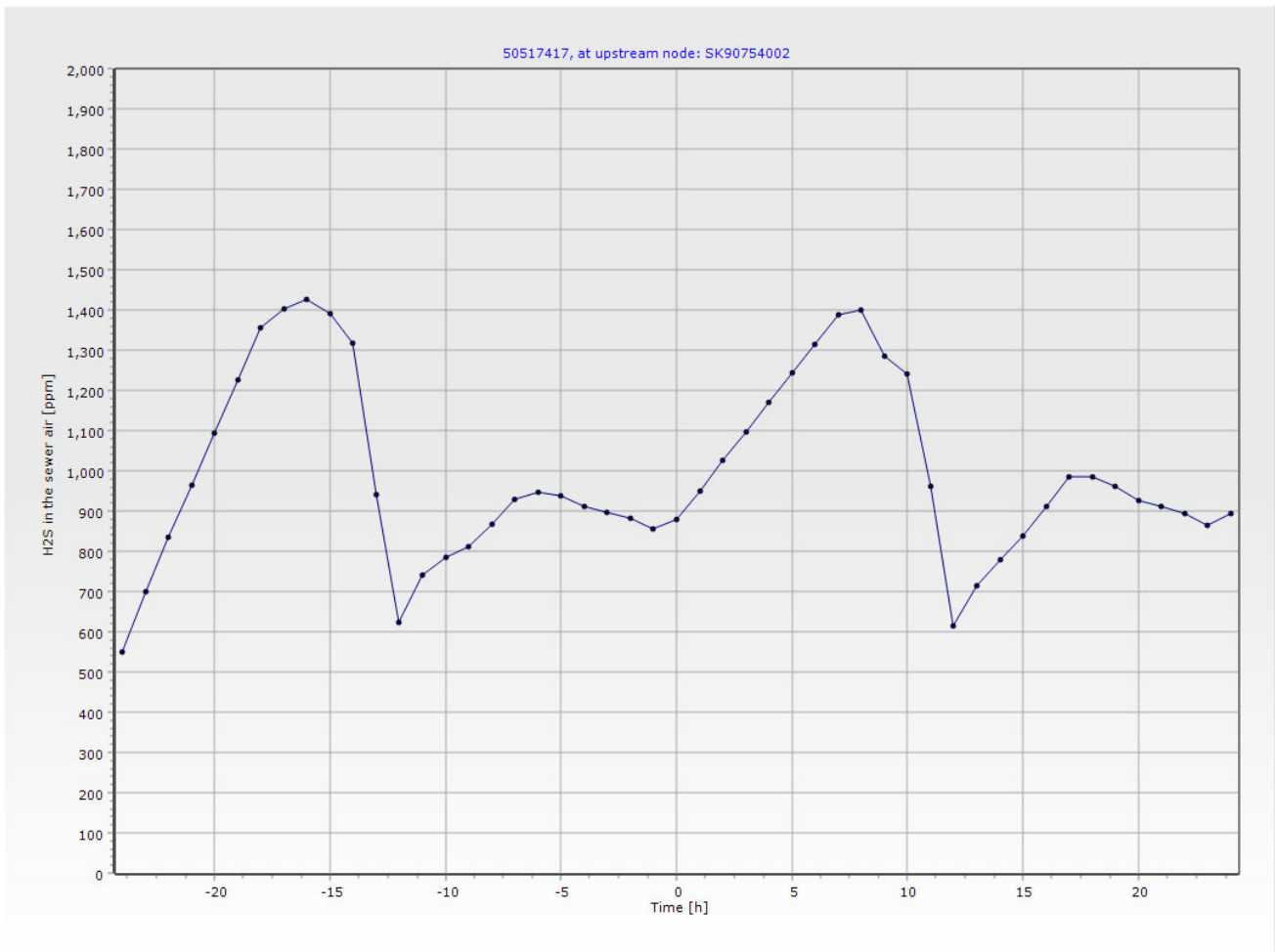


Figure 102. A diurnal simulation showing the simulated H<sub>2</sub>S-gas concentrations

Diurnal variations can be shown for the upstream node or the downstream node by checking or un-checking the checkbox below the pipe list box (*If checked show upstream values else show downstream*). If downstream values are chosen, the time scale on the time axis is the outlet of the force main. I.e. the time the water was sent on its way plus the travel time in the force main. The downstream graph shows the concentrations of the water plugs from the upstream node when they enter the downstream node.



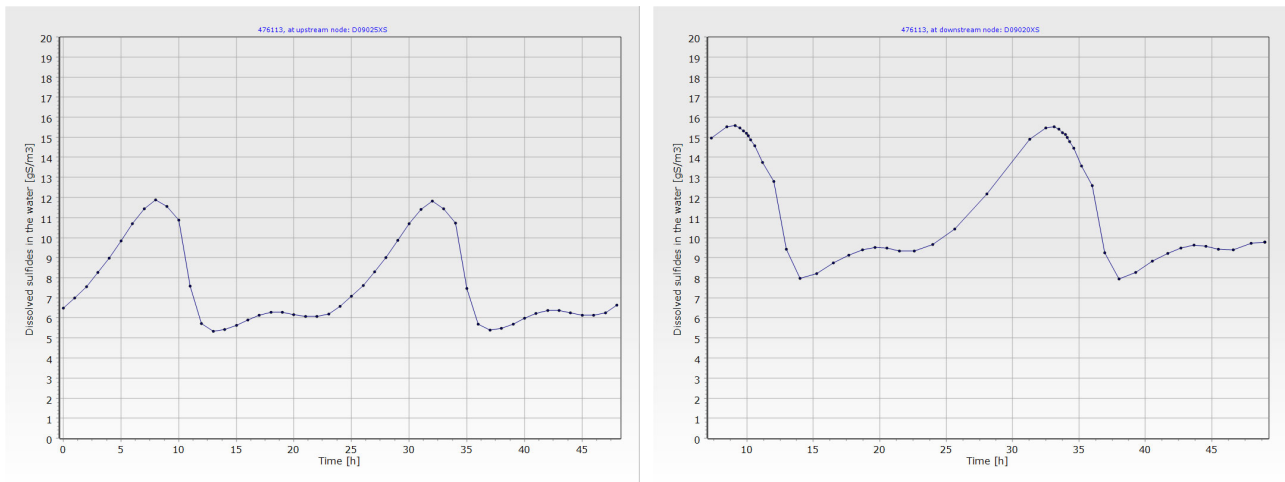


Figure 103. Upstream diurnal variation (left) and downstream diurnal variation of dissolved sulfide in a force main.

It is also possible to show flow paths for specific time steps of a diurnal variation pattern. This is done by setting the respective values in the *Default network and flow settings* (Figure 41). First chose *Length profile similar to average simulations – for a pre-defined time*. Then set the time step for which to show the parameters.

## 9 Defining model parameters

Mega-WATS holds a significant number of model parameters, which all are accessible through *Input → Set model parameters* form. The form holds several pages, as far as possible, organized into themes.

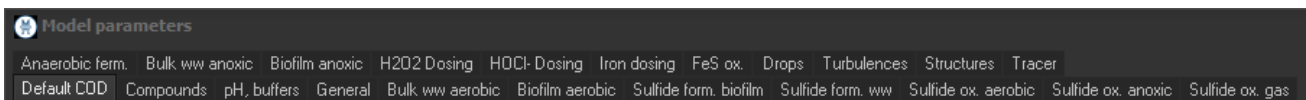


Figure 104. The pages of the model parameter form

### 9.1 COD Fractionation

Wastewater COD can be subdivided in various ways, for example total COD can be subdivided into what often is termed particulate, colloidal, and soluble COD by filtering on a membrane of pore size of, for example, 0.45  $\mu\text{m}$  and then flocculating what passes the filter. Particulate COD is the difference between total and filtered, colloidal COD is the difference between filtered and flocculated, and soluble COD is the flocculated value. Soluble COD can be further divided into fermentation substrate and product by measuring the volatile fatty acid content. Particulate COD, what is removed in the filter, can be divided into several relevant divisions based on bioavailability. For example, the fraction of inert particulates (fraction of COD which oxidizes too slowly to significantly influence transformations within a sewer environment) can be determined as the difference between Total COD and  $\text{BOD}_5$ . Bioavailable particulates are equal to the difference between particulate COD and inert particulates. Bioavailable particulates included the sum of biomass of several types and particulates which are hydrolysable to smaller, more readily bioavailable particles. There is no convenient test to fractionate the various biomass species and hydrolysable particulate.

A full fractionation can be done using oxygen uptake rate measurements, but the method is tedious and not available as standard analysis. However, typical biomass concentrations may be inferred based on sewage age.

COD fractions roughly correspond to particle size that are relevant because each reacts at different rates. Seen from the bacterial point of view, particles of several hundred nanometers are huge, as bacteria often have sizes in the order of a micrometer. The colloidal material, which includes small particles as well as larger molecules, cannot diffuse across the cell membrane and must be degraded outside the cell before taking up by the bacteria.

This was recognized early in the study of wastewater processes, and the IWA Activated Sludge Models first developed back in the 70s hence from the very beginning included a fractionation of the COD into groups relevant for the microbial processes. The core thinking is to divide the COD into

- a) The organisms who do the work, in this case the bacteria.
- b) The substrate which these bacteria can take up directly via diffusion over the cell wall.
- c) The substrates which need some sort of extracellular digestion (hydrolysis) into smaller substances, which then can be taken up over the cell membrane.
- d) Organic matter, which is inaccessible to the bacteria, i.e., inert organic material.

The sum of the above fractions yields the total COD of the wastewater.

The smart thing about using COD as the core of quantifying organic matter is that it is measured in the unit of potential oxygen consumption. COD measures how much oxygen (or better, how many electrons) are needed to oxidize organic matter into inorganic substances such as water, carbon dioxide, ammonia, phosphate, etc. Hence it is possible to put equations like  $\Delta\text{COD} = \Delta\text{O}_2$ , i.e., the change in total COD equals the amount of oxygen taken up. The principle can then be extended to COD oxidation by other electron acceptors, such as sulfate and nitrate.

Due to the nature of things, the Activated Sludge Models focus on what happens in a wastewater treatment plant. Treatment plants are characterized by having very high concentrations of biomass (which is what makes the sludge into activated sludge) and very little available organic substrate. This holds especially true for treatment plants targeting biological nutrient removal. Hence the bacteria tend to be substrate limited (i.e., they are starved).

Sewers, on the other hand, are seldom substrate limited and organic matter tends to be in surplus. Instead, they are limited by the available biomass and often also by available oxygen. This means that the processes taking place in sewers will differ from those in treatment plants. To acknowledge these (and other) differences in process conditions, the COD in sewers must be fractionated differently than COD in treatment plants. In principle the approach for sewers is the same as for an activated sludge process, but the COD fractionations are not the same. In other words, the fractions used in Mega-WATS are translatable to the fractions used in treatment plants models, but not identical to them.

### 9.1.1 Biomass

Mega-WATS includes both an attached growth reactor model, which pertains to the submerged biofilm living on the pipe walls, and a plug flow reactor model which pertains to the bulk flow. Each of four biomass groups are tracked. In the attached growth model, biomass abundance is represented in terms of the surface

area-to-volume ratio. While in the bulk flow each group are tracked by concentration. Each biomass group pertains, respectively, to the following important reactions:

- $X_{Hw}$  is the heterotrophic biomass which transforms organic matter under aerobic and anoxic conditions
- $X_{Hsulf}$  is sulfide forming biomass shed from the biofilm into the bulk water
- $X_{Hferm}$  is fermentative biomass shed from the biofilm into the bulk water
- $X_{Hch4}$  is methane forming biomass (methanogens) shed from the biofilm into the bulk water

Note that Mega-WATS does not contain any ammonia oxidizing biomass as no such biomass can exist under typical sewer conditions. Here the autotrophic ammonia oxidizers grow much slower than the heterotrophs and hence loose the competition for oxygen within the biofilm. Nevertheless, Mega-WATS allows nitrification to occur under conditions where degradable COD becomes depleted (section 9.4.12).

Model parameters

Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer

Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Default $X_{Hw}$ concentration and distribution	gCOD/m <sup>3</sup>	34.000	10.200	10.000	250.000	Fixed
Default $X_{Hsulf}$ concentration and distribution	gCOD/m <sup>3</sup>	0.000	0.000	0.000	10.000	Fixed
Default $X_{Hferm}$ concentration and distribution	gCOD/m <sup>3</sup>	0.000	0.000	0.000	10.000	Fixed
Default $X_{Hch4}$ concentration and distribution	gCOD/m <sup>3</sup>	0.000	0.000	0.000	10.000	Fixed
Default SF concentration and distribution	gCOD/m <sup>3</sup>	35.000	10.500	0.100	300.000	Fixed
Default SA concentration and distribution	gCOD/m <sup>3</sup>	12.000	3.600	0.100	300.000	Fixed
Default $X_{Sf}$ concentration and distribution	gCOD/m <sup>3</sup>	169.000	50.700	10.000	1500.000	Fixed
Default $X_{Sm}$ concentration and distribution	gCOD/m <sup>3</sup>	190.000	57.000	10.000	1500.000	Fixed
Default $X_{Ss}$ concentration and distribution	gCOD/m <sup>3</sup>	220.000	66.000	100.000	3500.000	Fixed
Default $X_{Si}$ concentration and distribution	gCOD/m <sup>3</sup>	15.000	4.500	0.000	4000.000	Fixed

Calculate new CODtotal

The total default COD in the wastewater is 675 g/m<sup>3</sup>

Modify COD fractions proportionally to a new total COD value of  g/m<sup>3</sup>

Figure 105. Default COD composition of wastewater entering the network

### 9.1.2 Organic substrates

Mega-WATS operates with five degradable substrate fractions:

- $S_F$  is fermentable organic substrate
- $S_A$  is fermentation products
- $X_{Sf}$  is fast hydrolysable substrate
- $X_{Sm}$  is medium hydrolysable substrate
- $X_{Ss}$  is slow hydrolysable substrate

$S_F$  is the organic fraction that can easily be fermented, covering for example sugars. In principle, this fraction is identical to the fraction of the same name in the activated sludge models. However, as the activated sludge models operate only with one hydrolysable fraction while Mega-WATS operates with three, the fast

hydrolysable fraction ( $X_{sf}$ ) of Mega-WATS would roughly be covered in the  $S_F$  fraction of the activated sludge models, while the medium and slow hydrolysable fractions ( $X_{sm}$  and  $X_{ss}$ ) of Mega-WATS would roughly correspond to the hydrolysable fraction of the activated sludge models. The exact division does however depend on the hydrolysis rate parameters and should be evaluated in detail when converting Mega-WATS COD fractions to fractions relevant for wastewater treatment plant models.

### 9.1.3 Inert organic matter

Mega-WATS operates with one inert organic matter fraction called  $X_{Si}$ . It here differs from activated sludge models which operate with a particulate and a soluble inert organic matter fraction. When converting between Mega-WATS COD fractions and wastewater treatment plant COD fractions,  $X_{Si}$  should be interpreted as covering the sum of these.

### 9.1.4 Setting COD values

The values of COD fractions and those of many other parameters can be set using the default buttons to the right of the parameter setup form. However, default values are meant to reflect 'typical' fresh municipal wastewater and should only be considered a starting point. Preferably, field sampling should be completed, and the input COD fractions should be selected to cause model agreement with measured values. Once that is accomplished COD fractions may be further refined for certain sewer network branches which are suspected to be different from the global wastewater quality, such as a restaurant districts, food processing plant or another industrial discharger.

Mega-WATS has some functions to facilitate the setting of COD fractions. They are found in the lower left part of the form (Figure 104).

- To modify all COD fractions at once, add a new total COD value in the input form (where there is written 675 in Figure 104) and then press the speed button (the one with the two hammers). Now all fractions are modified proportionally to the new total COD value.
- One can also change the fractions one by one. Press the button *Calculate new CODtotal* to see what the total COD of the manually added fractions amounts to.

## 9.2 pH and buffer system

Mega-WATS calculates the pH following an approach laid out in the IWA Anaerobic Digester Model No. 1, balancing the sum of anions and cations. It applies physico-chemical equations that describe ion association and dissociation as well as gas-liquid transfer of substances which affect the pH ( $\text{CO}_2$  and  $\text{H}_2\text{S}$ )

The parameters mainly associated with the pH and buffer system are accessible on the page *pH, buffers* (Figure 105). Note that most processes affect pH and the buffer system in one way or another, for example breakdown of COD forms carbonate, which then affects the buffer system, which then affects the pH.

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl-Dosing Iron dosing FeS ox. Acid-base Drops Turbulences Structures Tracer Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Default pH values and pH distribution	-	7.800	1.000	6.000	9.000	Fixed
Default pCO <sub>2</sub> g concentration in air intake from atmosphere (accounts also for CO <sub>2</sub> formation in laterals)	ppm CO <sub>2</sub> gas	1000	300	400	12000	Fixed
Default dissolved carbonate concentration and distribution	mol/L	0.003500	0.001750	0.000100	0.010000	Fixed
Default NH <sub>3</sub> total concentration and distribution	mol/L	0.002565	0.001283	0.000357	0.007143	Fixed
Default amino groups concentration and distribution	mol/L	0.002835	0.001417	0.000500	0.010000	Fixed
Default PO <sub>4</sub> total concentration and distribution	mol/L	0.000155	0.000078	0.000023	0.022581	Fixed

Figure 106. Parameters mainly associated with pH and the buffer system

The parameters accessible are:

- Default pH is the pH at the wastewater source.
- Default pCO<sub>2</sub>g is the concentration of CO<sub>2</sub>-gas in air entering the sewer together with sewage. One can also view this as the CO<sub>2</sub>-concentration in the very upstream end of the sewer network
- Dissolved carbonate is the sum of carbonate species (H<sub>2</sub>CO<sub>3</sub>, HCO<sub>3</sub><sup>-</sup>, and CO<sub>3</sub><sup>2-</sup>) in the system, the distribution of which between individual chemical species depends on the pH. The pKa-values of the carbonate system are accessible on the same page (Figure 109).
  - Note that the pH can rapidly change if there is an dis-equilibrium between the CO<sub>2</sub>-gas dissolved in the wastewater and headspace gas CO<sub>2</sub> concentration. The interaction between the two phases strongly affects pH. Examples are given in Figure 106, Figure 107, and Figure 108. In Figure 106, the carbonate system of the wastewater is quite far from equilibrium as the water is super-saturated. CO<sub>2</sub> is hence released, increasing both pH and sewer headspace CO<sub>2</sub>. In Figure 107, The initial CO<sub>2</sub> concentration of the headspace is increased, and the carbonate content decreased, while pH is kept the same. This leads to the water and air phases being close to equilibrium. Changes hence happen slowly. In Figure 108, the same conditions as in Figure 107 are applied, but for pH being increased to 8.0. This leads to under-saturated wastewater, and CO<sub>2</sub> transfers from the air to the water, causing decreases in pH and CO<sub>2</sub> headspace concentrations.
- NH<sub>3</sub>total is the total ammonia concentration, i.e., ammonium plus ammonia. It is not affected by any processes but affects the buffer system when pH is above approximately 8. For example, ammonia contributes the cost of dosing alkaline chemicals to raise pH. The pKa-value of the ammonia system is accessible on the same page (Figure 109).
- Amino groups are associated with organic matter and affect the cost of pH adjustment similarly to ammonia. The pKa value of amino groups differ between substances, and a single value is used to represent this category of constituent (Figure 109) based on experiments with titrating wastewater with hydroxide.
- PO<sub>4</sub>total is the phosphate content of the wastewater. In practice it has limited influence on the pH.

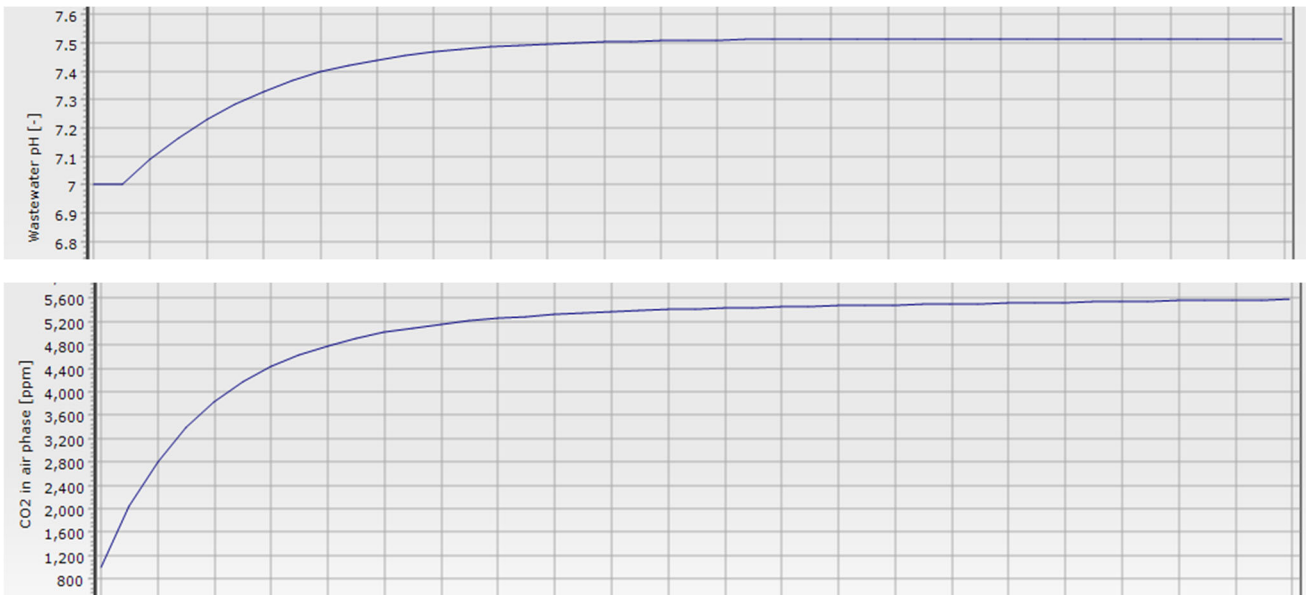


Figure 107. pH and CO<sub>2</sub>-gas in and upstream pipe with little flow. The wastewater initially contains 1000 ppm CO<sub>2</sub>-gas content and 3.5 mM dissolved carbonate. Initial pH is 7.0

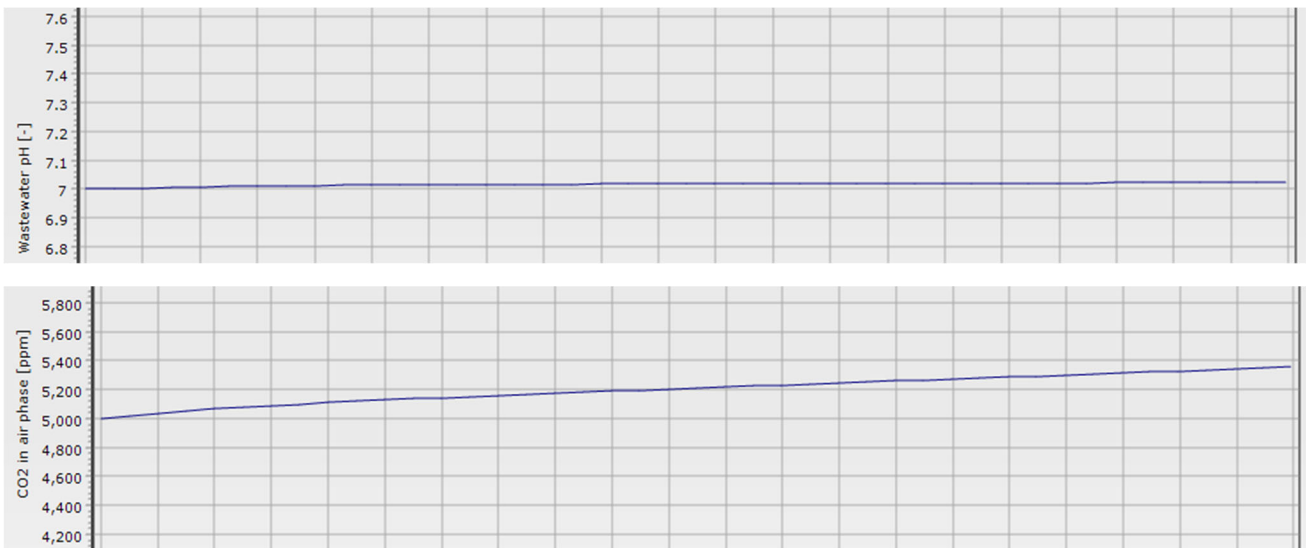
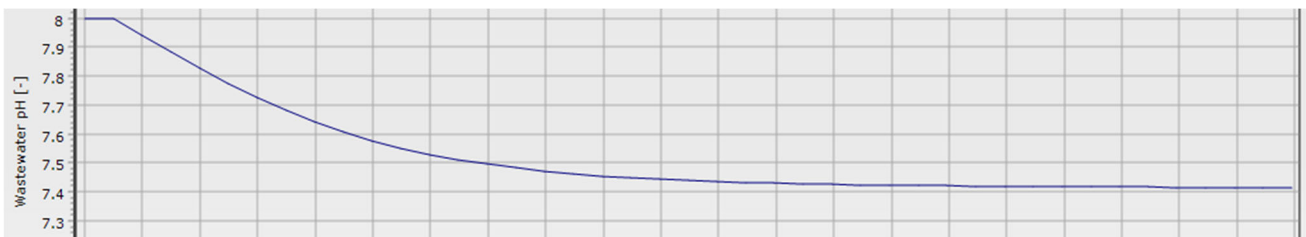


Figure 108. pH and CO<sub>2</sub>-gas in and upstream pipe with little flow. The wastewater initially contains 1000 ppm CO<sub>2</sub>-gas content and 1.0 mM dissolved carbonate. Initial pH is 7.0





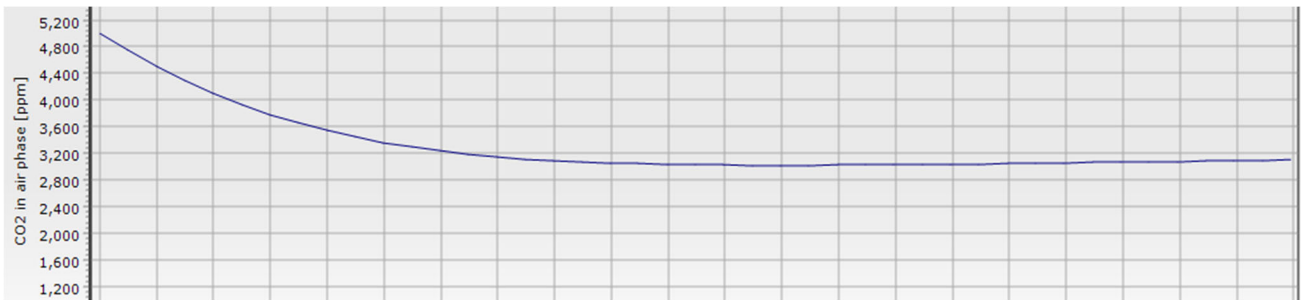


Figure 109. pH and CO<sub>2</sub>-gas in and upstream pipe with little flow. The wastewater initially contains 1000 ppm CO<sub>2</sub>-gas content and 1.0 mM dissolved carbonate. Initial pH is 8.0

The acid-base constants of other relevant substances are also accessible on the pH, buffers page (Figure 109), some more important than others, and some should probably not be changed.

This page also gives access to the solubility product of magnesium hydroxide, which is in play when dosing magnesium hydroxide to increase wastewater pH.

	pKa1]	pKa2]	pKa3]		pK <sub>sp</sub>
Carbonic acid dissociation constants	6.38	10.32	-	Solubility product, Magnesium Hydroxide	11.251
Acetic acid dissociation constant)	4.76	-	-		
Hydrogen sulfide dissociation constants	7.05	14.00	-		
Phosphate dissociation constants	2.12	7.21	12.67		
Ammonia dissociation constant)	9.21	-	-		
Amino groups dissociation constant)	9.50	-	-		
Sulfuric acid (2) (HSO <sub>4</sub> <sup>-</sup> ) dissociation constant)	1.92	-	-		
Nitric acid (NO <sub>3</sub> <sup>-</sup> ) dissociation constant)	-1.30				

Figure 110. Acid-base physico-chemical parameters

### 9.3 General parameters

The page Global parameters holds a mix of parameters (Figure 110).

- Temperature. Mega-WATS operates at a fixed temperature for the whole network
- Space step of the simulations. Typically, a space step of 1 m is suitable, i.e., values are calculated in a pipe for each meter. Increasing the space step can rapidly lead to increased numerical noise. Decreasing it reduces simulation noise, however, at the cost of increased calculation time. If simulations show bizarre results in the very upstream end of the system, a decrease in space step might solve such issue.
- Maximum time step of the simulation. The time step is calculated from the space step and the flow velocity from  $\Delta x / \Delta t = v$ , where  $v$  is the water velocity,  $\Delta x$  the space step and  $\Delta t$  is the time step. If the flow velocity is very low, this might lead to time steps that cause instability. There is hence a lower limit on the velocity. Decreasing this value can solve instability problems in pipes with very slow flow.
- Equivalent sand roughness of the pipe above the water governs the pipe wall friction on the air movement. It is a parameter governing of the air flow friction as described in section 13.1.

- Water surface drag coefficient governs the drag that the flowing water can assert on the sewer air. It is a parameter governing of the air flow drag as described in section 13.1.

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl-Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default COD Compounds pH, buffers <b>General</b> Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Temperature (T)	°C	22.00	2.00	0.00	100.00	Fixed
Space step of the calculations. A smaller space step reduces noise.	m	1.00	0.00	0.01	10.00	Fixed
Max time step of the calculations. A smaller step increases accuracy.	s	60	0	1	1000	Fixed
Equivalent sand roughness above the water line	m	0.00100	0.00025	0.00010	0.01000	Fixed
Water surface drag coefficient on air phase	-	0.007550	0.001888	0.000755	0.075500	Fixed
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Difference in reaeration rate, wastewater to clean water (alpha_rea)	-	1.00	0.10	0.50	2.00	Fixed
Difference in DO saturation concentration, wastewater to clean water (beta_rea)	-	1.00	0.10	0.50	2.00	Fixed
Arrhenius constant for reaeration (alpha_r)	-	1.030	0.010	1.000	1.100	Fixed
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Factor offsetting total COD, works on inlet COD to each node. All flow in one run is offset by same factor	-	1.000	0.300	0.200	10.000	Fixed
Factor offsetting total flow, works on inlet flow to each node. All flow in one run is offset by same factor	-	1.000	0.300	0.200	10.000	Fixed
Factor offsetting total pH, works on inlet flow to each node. All pH in one run is offset by same factor	-	1.000	0.120	0.780	1.330	Fixed

Figure 111. General parameters

## 9.4 Biological and chemical processes

### 9.4.1 Biological bulk water processes, general considerations

Bulk water biological processes are controlled by the amount of biomass, its substrates, and conditions limiting process rates. Like in the activated sludge models and anaerobic digester models, most biological bulk water process rates are described as first order processes with respect to biomass. The growth of biomass under aerobic conditions, for example, is described by a first order process in the biomass. In case there are no substrate limitations, the process rate in principle is:

$$\frac{dX_H}{dt} = \mu_{max} X_H$$

Where  $X_H$  = Heterotrophic aerobic biomass  
 $t$  = time  
 $\mu_{max}$  = Maximum growth rate of  $X_H$

However, there are nearly always some limitations. Oxygen, for example. These are described by Michaelis–Menten kinetics (Monod kinetics). Including oxygen, this leads to:

$$\frac{dX_H}{dt} = \mu_{max} \frac{S_O}{K_O + S_O} X_H$$

Where  $S_O$  = Dissolved oxygen  
 $K_O$  = Saturation constant (half-velocity constant) for oxygen

Adding further limiting substrates, for example organic substrate, extends the equation to:

$$\frac{dX_H}{dt} = \mu_{max} \frac{S_O}{K_O + S_O} \frac{S_S}{K_S + S_S} X_H$$

Where  $S_S$  = Readily biodegradable substrate  
 $K_S$  = Saturation constant (half-velocity constant) for readily biodegradable substrate

Temperature also affects the process rates and are described by an Arrhenius equation. Also including a pH dependency leads to:

$$\frac{dX_H}{dt} = \mu_{max} \frac{S_O}{K_O + S_O} \frac{S_S}{K_S + S_S} X_H \alpha_w^{T-20} k_{H,pH}$$

Where  $\alpha_w$  = An Arrhenius constant  
 $T$  = The temperature of the wastewater  
 $k_{H,pH}$  = a function that limits the growth depending on pH

These equations are then extended until they encompass all substances and process limitations considered necessary.

Hydrolysis rates are described in a slightly different way, namely for example hydrolysis under aerobic conditions:

$$\frac{dX_{Sf}}{dt} = k_{hf} \frac{\frac{X_{Sf}}{X_H}}{K_{Xf} + \frac{X_{Sf}}{X_H}} \frac{S_O}{K_O + S_O} X_H \alpha_w^{T-20} k_{H,pH}$$

Where  $k_{hf}$  = Aerobic hydrolysis rate constant for fast hydrolysable matter  
 $K_{Xf}$  = Saturation constant  
 $X_{Sf}$  = Fast hydrolysable matter

While the fraction including the hydrolysable organic matter appears to be Michaelis–Menten kinetics, it is not. This is easily seen from the fact that the unit of  $K_{Xf}$  is  $\text{gCOD gCOD}^{-1}$ , and not  $\text{gCOD m}^{-3}$ , as it for example is for  $K_S$ . This equation is widely used in activated sludge modelling and is based on some theoretical considerations on how hydrolysis behaves. In practice, its main virtue is that it creates a fluid transition between the case where biomass limits the hydrolysis and where hydrolysable substrate limits it.

In addition to kinetics, mass balances are made in each compound. In the case of aerobic growth on readily biodegradable substrate, for example, as substrate and biomass are measured in COD (i.e., negative oxygen):

$$\Delta X_H + \Delta S_S + \Delta(-S_O) = 0$$

And it is assumed that a biological process occurs with a certain (fixed) yield:

$$Y_H = \frac{\Delta X_H}{\Delta S_S}$$

Where  $Y_H$  = Heterotrophic aerobic yield constant

Combining the stoichiometry of all involved processes and rates leads to formulation of the full WATS concept.

The above is but a small introduction to the full set of bulk water processes behind Mega-WATS. The complete set of stoichiometric and rate expressions are provided in the document *WATS matrix*.

#### 9.4.2 Aerobic bulk water processes

The parameters for the aerobic bulk water process are accessible via the page *Bulk ww aerobic* of the *Model parameters* form (Figure 111).

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCI- Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Maximum growth rate of the heterotrophic biomass at 20°C (my)	1/d	6.00	2.00	2.00	15.00	Fixed
Yield constant for bulk water aerobic heterotrophic biomass (YHwO2)	mol e-eq/mol e-eq	0.550	0.050	0.300	0.800	Fixed
Saturation constant for readily biodegradable substrate (KS)	gCOD/m3	1.00	0.20	0.10	10.00	Fixed
Saturation constant for dissolved oxygen (KO)	gO2/m3	0.100	0.050	0.010	1.000	Fixed
Maintenance energy rate constance at 20°C (qm)	1/d	0.500	0.200	0.100	2.000	Fixed
Minimum maintenance energy rate constance at 20°C (qmMin)	1/d	0.125	0.050	0.025	0.500	Fixed
Rate constant for fast hydrolysable substrate at 20°C (kh,fast)	1/d	4.000	1.200	1.000	15.000	Fixed
Saturation constant (KX,fast) for kh,fast depends on kh,fast with the slope (no dependency = zero)	gCOD/gCOD	0.230	0.050	0.050	1.000	Fixed
and with the intersection (if no dependency, then this is equal to KX,fast)	gCOD/gCOD	-0.500	0.100	-1.000	-0.001	Fixed
Rate constant for medium hydrolysable substrate at 20°C (kh,med)	1/d	1.000	0.500	0.500	3.000	Fixed
Saturation constant (KX,med) for kh,med depends on kh,med with the slope (no dependency = zero)	gCOD/gCOD	0.230	0.050	0.000	1.000	Fixed
Saturation constant (KX,med) for kh,med depends on kh,med with the slope (no dependency = zero)	gCOD/gCOD	-0.500	0.100	-1.000	-0.001	Fixed
Rate constant for slow hydrolysable substrate at 20°C (kh,slow)	1/d	0.50	0.30	0.10	3.00	Fixed
Saturation constant for slow hydrolysable substrate (KX,slow)	gCOD/gCOD	0.900	1.300	0.010	5.000	Fixed
Arrhenius constant for the bulk water heterotrophic transformations (alpha_w)	-	1.070	0.010	1.000	1.150	Fixed
Parameter accouting for the width of the biological heterotrophic pH dependency	-	175.00	20.00	20.00	1000.00	Fixed

Figure 112. Aerobic bulk water process parameters

#### 9.4.3 Biological biofilm processes, general considerations

The substrates, for example oxygen, are present in the bulk water of the sewer. They then become transformed either in the bulk water or the biofilm below the water line. To be consumed in the biofilm, the substrates must get from the bulk water and into the biofilm.

The bulk water can be described as completely mixed, as Reynolds numbers are quite high (conditions are highly turbulent). The biofilm, on the other hand, is a slimy layer containing biomass, extracellular polymeric substances (EPS), and particles from the wastewater that have been caught in the biofilm matrix. The dry matter content of a sewer biofilm depends on the conditions in the sewer, where anaerobic biofilms in force mains for example differ from aerobic biofilms in gravity sewers. Typical densities are somewhere around

20-80 kg dry matter per m<sup>3</sup> of biofilm, with thicknesses in gravity mains around 1-1.5 mm, and somewhat thinner in force mains.

Inside the biofilm, the water tends to be quiescent, as the solid matrix would impose high energy losses on convective water flows. Transport of substances is hence driven by diffusion. Between the completely mixed bulk water and the biofilm there will be a diffuse boundary layer where the velocity at on the biofilm side will be zero and at the bulk water side will be the velocity of the flowing water. For modelling purposes, this boundary layer can be assumed quiescent and containing no biomass.

Applying biofilm diffusion kinetics as described by Fick's first law:  $J = -A_f D_w \frac{\partial S}{\partial x}$

where:

- $J$  = Flux of substrate in the x-direction
- $A_f$  = Cross-sectional area of biofilm through which the flux occurs
- $D_w$  = Molecular diffusion coefficient of the substrate S in water
- $S$  = Substrate concentration
- $x$  = Distance

together with the transformation of substrates like what happens in the bulk water, the concentration of substances in the film can be described. An example of such modelling is shown in Figure 112.

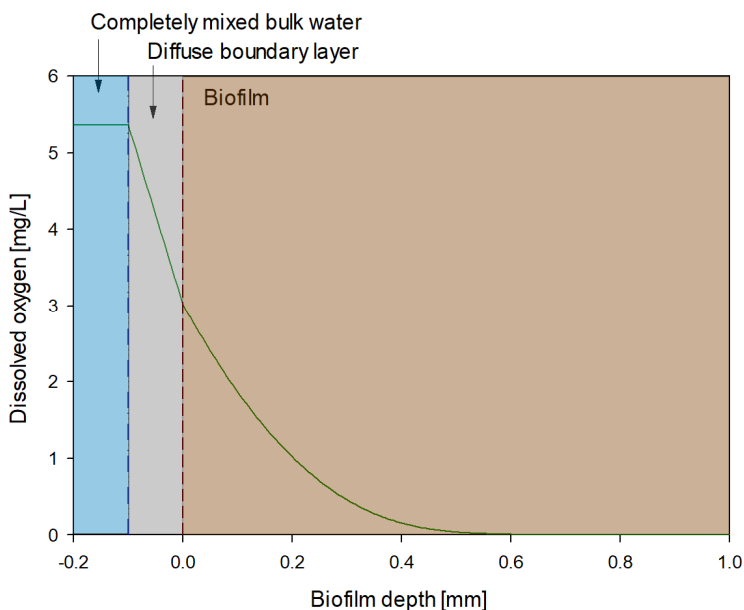


Figure 113. Modelling of dissolved oxygen in a biofilm. The model is a 1-D model assuming a homogeneous biofilm thickness and composition in the (x,y)-directions. The only substance limiting the transformation rate is oxygen.

In the simulation of Figure 112, only oxygen is limiting the biological transformations. Organic matter (readily degradable substrate) is present at non-limiting concentrations. Furthermore, the biofilm is seen to be partly penetrated by oxygen, as it does not reach to the bottom of the film. Below approx. 0.5 mm, the biofilm is anaerobic. Increasing or decreasing the oxygen concentration in the bulk water would lead to a corresponding increase or decrease in oxygen penetration depth into the biofilm. If the biofilm is not fully penetrated, that change will be non-linear in the bulk water dissolved oxygen concentration. Figure 113 illustrates this by showing the oxygen profile for three different bulk water concentrations.

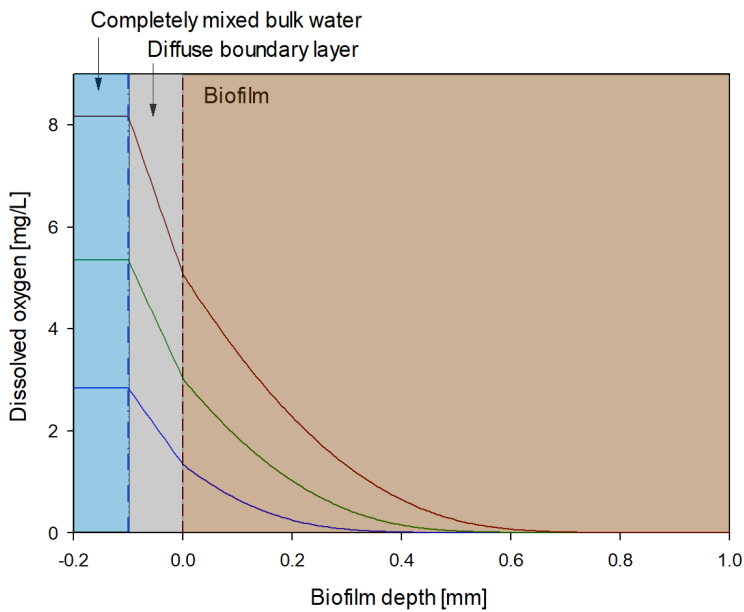


Figure 114. Modelling of dissolved oxygen in a biofilm at three different concentrations in the bulk water. The model is a 1-D model assuming a homogeneous biofilm thickness and composition in the (x,y)-directions. The only substance limiting the transformation rate is oxygen.

Under certain simplifying conditions, explicit solutions can be found that express the oxygen uptake rate of the biofilm in terms of the oxygen concentration in the bulk water. Assumptions: Transformations inside the biofilm are of first order in the biomass inside the film; Transformation of substrates are of zero-order; Only one substrate limits the transformations; The biomass concentration inside the film is constant and independent on the depth at which the transformations occur; The biofilm thickness remains constant.

The set of equations can be solved for two conditions:

- The biofilm is partly penetrated by the substrate in question. This leads to the bulk water substrate uptake rate following a half-order process rate in the bulk water concentration:

$$\frac{dS_{x,w}}{dt} = k_{x,1/2} S_{x,w}^{1/2}$$

Where  $S_{x,w}$  is the concentration of a substrate in the bulk water, for example oxygen ( $S_O$ ),  $k_{x,1/2}$  is a half order rate constant, and  $t$  is time.

- The biofilm is fully penetrated by the substrate in question. This leads to the bulk water substrate uptake rate following a zero-order process rate in the bulk water concentration:

$$\frac{dS_{x,w}}{dt} = k_{x,0} S_{x,w}^0 = k_{x,0}$$

Where  $k_{x,0}$  is a zero-order rate constant.

In other words, when a biofilm is partly penetrated, the rate by which the biofilm removes substrate from the bulk water is a half order function in the water phase substrate concentration. When a biofilm is fully penetrated, the rate by which the biofilm removes substrate from the bulk water is a constant.

This approach assumes that only one substrate is limiting at the time, which commonly is a reasonable assumption. Aerobic heterotrophic processes, for example, can be limited by either oxygen or by the



available substrate. However, it is the exception that both limitations occur simultaneously, and should this occur, it would be only for a short period, and would not induce significant error in the model.

In recognition of the film sometimes becoming fully penetrated, the half order rate function is only assumed valid up to some maximum water phase concentration, upon which it becomes constant, i.e., following a zero-order process rate. The general shape of how a biofilm process is simulated in Mega-WAS is shown in Figure 114. Details on how to derive at these equations can be found in many textbooks and articles on biofilm process kinetics, for example Harremoës (1978), Characklis and Marshall (1990), and Jansen et al. (2021).

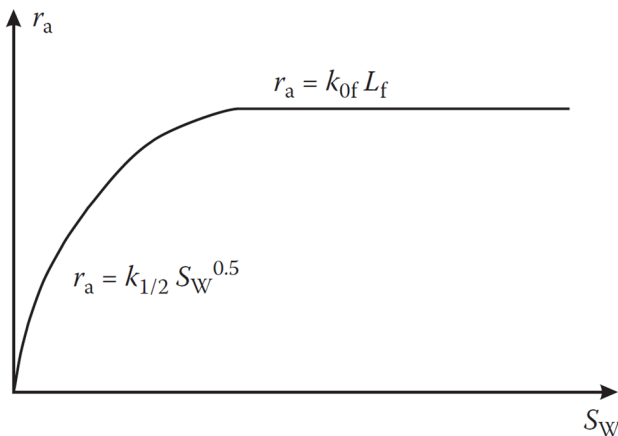


Figure 115. General shape of biofilm rate functions in Mega-WATS

Mega-WATS assumes that the biofilm is in steady state, and that the biomass produced in the biofilm is continuously released to the bulk water.

For non-ideal situations, a model like the one used in Figure 112 and Figure 113 can be applied to model details of biofilm processes. However, such model is quite calculation intensive, and using it for sewer process modelling would slow down the simulations by many orders of magnitude. For this reason, Mega-WATS applies the outcome of the explicit solution to biofilm kinetics.

#### 9.4.3.1 Including biofilm kinetics in the Mega-WATS model matrix

The rate expressions for the biofilm process are in units of the substrate in question, for example oxygen. The unit is for example  $\text{g-O}_2 \text{ m}^{-2} \text{ h}^{-1}$ . The concentration in the bulk water is, however, in  $\text{g-O}_2 \text{ m}^{-3}$ , and the transformation rate consequently  $\text{g-O}_2 \text{ m}^{-3} \text{ h}^{-1}$ . A conversion from surface uptake rate to the corresponding bulk water removal rate is hence needed.

Denote the biofilm uptake rate by  $r_f$  ( $\text{gO}_2 \text{ m}^{-2} \text{ h}^{-1}$ ), the biofilm area of a pipe of length  $L$  [m] by  $A_f$  [ $\text{m}^2$ ], and the corresponding water volume of the pipe by  $V_w$  [ $\text{m}^3$ ].

Converting from the biofilm uptake rate to the experienced removal of oxygen in the bulk water ( $r_w$ ,  $\text{gO}_2 \text{ m}^{-3} \text{ h}^{-1}$ ) becomes:

$$r_w = r_f \frac{V_w}{A_f}$$

In addition, the basis of the Gujer matrix used to describe the processes in Mega-WATS is the biomass, as this is the active agent in the conversion processes. To convert from a substrate, in this example dissolved oxygen, to the biomass produced, the stoichiometry of the process must be established as for example:

$$\Delta X_H + \Delta S_S + (-\Delta S_O) = 0$$

The unit of  $X_H$  and  $S_S$  is  $\text{gCOD m}^{-3}$  and the unit  $S_O$  is  $\text{gO}_2 \text{m}^{-3}$ . Recalling that COD is the oxygen needed to reduce organic matter to inorganic substances ( $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , ...) and that COD hence is the potential to consume oxygen, explains why COD and  $\text{O}_2$  have opposite signs.

While consuming oxygen, the biomass is growing. This process is quantified by the yield ( $Y_H$ ):

$$Y_H = -\frac{\Delta X_H}{\Delta S_S}$$

The reason for the minus sign is that when  $X_H$  increases,  $S_S$  decreases, and it is preferred to have  $Y_H$  positive.

From these two equations one can deduct the relationship between  $X_H$ ,  $S_S$ , and  $S_O$ :

$$\Delta S_S = \frac{-1}{Y_H} \Delta X_H$$

$$-\Delta S_O = \frac{1 - Y_H}{Y_H} \Delta X_H$$


In other words, for each gram of biomass produced, there is used  $1/Y_H$  gram of  $S_S$  and  $(1-Y_H)/Y_H$  gram of  $S_O$ .

Similarly, converting from oxygen consumed by the biofilm to biomass produced by the biofilm and then released to the bulk water becomes:

$$\Delta X_H = -\frac{Y_H}{1 - Y_H} \Delta S_O$$

#### 9.4.4 Aerobic biofilm processes

The parameters for the aerobic biofilm process are accessible via the page *Biofilm aerobic* of the *Model parameters* form (Figure 115).



Parameter	Unit	Mean	StDev	Min	Max	Distribution
½ order rate constant for biofilm, aerobic conditions [k½O2]	(gO2/m)½ 1/d	6.000	2.000	2.000	100.000	Fixed
Yield constant for biofilm biomass, aerobic conditions [YHfO2]	gCOD/gCOD	0.550	0.050	0.400	0.800	Fixed
Saturation constant for biofilm organic substrate	gCOD/m3	4.00	2.00	0.10	20.00	Fixed
Biofilm biomass efficiency constant (epsilon)	-	0.30	0.10	0.10	0.60	Fixed
Biofilm biomass concentration [XB, film]	gCOD/m2	10.0	1.0	1.0	100.0	Fixed
Arrhenius constant for the biofilm heterotrophic transformations (alpha_f)	-	1.050	0.010	1.000	1.100	Fixed

Figure 116. Aerobic biofilm process parameters

#### 9.4.5 Hydrolysis

Hydrolysis occurs under aerobic, anoxic, and anaerobic conditions. The rates under the two latter conditions are assumed a fraction of the rate under aerobic conditions. The rate fraction for anaerobic hydrolysis is set on the *Anaerobic ferm.* page (Figure 121), row *Anaerobic hydrolysis efficiency constant*. For anoxic hydrolysis, it is set on the *Bulk ww anoxic* page (Figure 122), row *Relative hydrolysis under anoxic conditions compared to aerobic conditions*.

Hydrolysis occurs in both the bulk water and biofilm.

Hydrolysis in Mega-WATS covers three fractions of hydrolysable matter: fast, medium, and slow hydrolysable matter. Each is transformed at its own rate to fermentable substrate (section 9.1.2)

Hydrolysis rates are described in a slightly different way, namely, for example, fast hydrolysable matter under aerobic conditions in the bulk water:

$$k_{hf} \frac{\frac{X_{Sf}}{X_H}}{K_{Xf} + \frac{X_{Sf}}{X_H}} \frac{S_O}{K_O + S_O} X_H \alpha_w^{T-20} k_{H,pH}$$

Where

- $\alpha_w$  = An Arrhenius constant
- $\mu_{max}$  = Maximum growth rate of  $X_H$
- $k_{hf}$  = Aerobic hydrolysis rate constant for fast hydrolysable matter
- $k_{H,pH}$  = a function that limits the growth depending on pH
- $K_O$  = Saturation constant (half-velocity constant) for oxygen
- $K_S$  = Saturation constant (half-velocity constant) for readily biodegradable substrate
- $K_{Xf}$  = Saturation constant
- $S_S$  = Readily biodegradable substrate
- $S_O$  = Dissolved oxygen
- $T$  = The temperature of the wastewater
- $X_H$  = Heterotrophic aerobic biomass
- $X_{Sf}$  = Fast hydrolysable matter

The rate in the biofilm for the same fraction and same electron acceptor conditions is:

$$k_{hf} \frac{\frac{X_{Sf}}{X_H}}{K_{Xf} + \frac{X_{Sf}}{X_H}} \frac{S_O}{K_O + S_O} \varepsilon_{Hf} X_{Hf} \frac{A_f}{V_w} \alpha_f^{T-20} k_{H,pH}$$

Where

- $\alpha_f$  = An Arrhenius constant
- $\varepsilon_{Hf}$  = An efficiency constant
- $A_f$  = Area of biofilm
- $V_w$  = Volume of water
- $X_{Hf}$  = biomass in the biofilm

#### 9.4.6 Sulfide formation

Sulfide formation occurs under anaerobic conditions and mainly in the biofilm and sediments of sewers as the growth rate of the sulfide forming organisms is comparatively slow. However, as the thickness of sewer biofilms (and sediments) on average stays constant, they shed biomass as they grow. This leads to sulfide

forming biomass in the bulk water, where the biomass may continue its growth, albeit seldom reaching significant concentrations. The details of the processes are given in the file *WATS matrix*, which is an addendum to this manual. The parameters for these processes are entered in the grids shown in Figure 116 and Figure 117.

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl-Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Hydrogen sulfide formation rate constant on SF(+SA) (kH2S)	(mgH2S/(m2h))^0.5	15.00	4.50	2.00	100.00	Fixed
Fraction of kH2S when using XF as sulfide formation substrate	-	0.100	0.030	0.010	0.100	Fixed
Saturation inhibition constant for biofilm sulfide formation in the presence of oxygen (KoH2Sf)	gO2/m3	0.100	0.010	0.001	1.000	Fixed
Saturation inhibition constant for biofilm sulfide formation in the presence of nitrate/nitrite (KNOH2Sf)	gN/m3	0.200	0.020	0.002	2.000	Fixed
Saturation inhibition constant for biofilm sulfide formation with respect to sulfate (KSO4f)	gS/m3	3.00	0.30	0.03	30.00	Fixed
Arrhenius constant for the H2S emission (alpha_rs)	-	1.030	0.010	1.000	1.100	Fixed
Arrhenius constant for the biofilm sulfide formation (alpha_s)	-	1.030	0.010	1.000	1.100	Fixed
Yield constant for growth on SA+SF and sulfate when forming sulfides	(gCOD/gCOD)	0.500	0.100	0.100	0.700	Fixed
The fraction of SF to SA used when forming sulfide	m	1.000	0.100	0.000	1.000	Fixed
Parameter	Unit	Mean	StDev	Min	Max	Distribution
The factor by which kH2S increases in the presence of sediments	-	2.00	0.50	1.00	5.00	Fixed
The sediment depth above which kH2S increases due to sediments	m	0.010	0.001	0.000	1.000	Fixed
The factor by which to multiply kH2S to get kH2S at zero shear (gravity main)	-	0.00	0.25	0.00	1.00	Fixed
The "monod" constant making a smooth shift from thauZero*kH2S to kH2S (gravity main)	-	0.00	0.20	0.00	2.00	Fixed
The factor by which to multiply kH2S to get kH2S at zero shear (force main)	-	0.00	0.20	0.00	1.00	Fixed
The "monod" constant making a smooth shift from thauZero*kH2S to kH2S (force main)	-	0.00	0.20	0.00	2.00	Fixed

Figure 117. Sulfide formation in biofilms and sediments

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl-Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Maximum growth rate of sulfate reducing biomass in bulk water at 20°C (my)	1/d	0.50	0.02	0.01	2.00	Fixed
Saturation inhibition constant for bulk water sulfide formation in the presence of oxygen (KoH2Sw)	gO2/m3	0.050	0.005	0.001	0.500	Fixed
Saturation inhibition constant for bulk water sulfide formation in the presence of nitrate/nitrite (KNOH2Sw)	gN/m3	0.100	0.010	0.001	1.000	Fixed
Saturation inhibition constant for bulk water sulfide formation with respect to sulfate (KSO4w)	gS/m3	0.50	0.05	0.01	5.00	Fixed
Decay rate constant for sulfate reducers (bXSulf)	d-1	0.50	0.05	0.01	5.00	Fixed

Figure 118. Sulfide formation in wastewater

#### 9.4.6.1 Dependency of sulfide formation on flow

As default, the sulfide formation is assumed independent on flow conditions. However, this is only partly correct, as sulfide formation in quiescent water is lower than in water flowing at some velocity. Hence it is possible for the user to change this in the last four rows of the input grid of Figure 116.

- Fraction of sulfide formation rate ( $r/r_{max}$ ) at zero shear stress (between 0 and 1) (gravity main)
- Saturation constant shifting from the zero shear to indefinite shear (gravity main)
- Fraction of sulfide formation rate ( $r/r_{max}$ ) at zero shear stress (between 0 and 1) (force main)
- Saturation constant shifting from the zero shear to indefinite shear (force main)

The parameter that governs the turbulence that the biofilm experiences is the pipe wall shear stress ( $\tau$  [Pa]), defined as:

$$\tau = \gamma RI$$

Where  $\gamma$  is the specific weight (density times gravity, [N/m<sup>3</sup>]),  $R$  is the hydraulic radius [m] and  $I$  the slope of the energy gradient [m/m].

Alternatively, one can think of this parameter as related to the shear velocity ( $u_*$  [m/s]):

$$u_* = \sqrt{\tau/\rho}$$

Where  $\rho$  is the density of the fluid.

A common error is to relate the dependency of a biofilm activity (such as the sulfide formation rate) to the average flow velocity of the water. The reason why this is fundamentally wrong, is that the biofilm solely experiences the rate of velocity change at its surface, i.e., the gradient of the velocity profile at the interface between liquid and biofilm, and not the average flow rate of the liquid.

It is possible to apply one set of parameters for gravity mains and one set for force mains. The relationship is:

$$r = r_{max} \left( k_{\tau_0} + \frac{\tau}{K_{\tau} + \tau} (1 - k_0) \right)$$

Where  $k_{\tau_0}$  is the fraction of sulfide formation rate ( $r/r_{max}$ ) at zero shear stress;  $K_{\tau}$  is the saturation constant shifting from the zero shear to indefinite shear. An example of how the formular plots is shown in Figure 118.

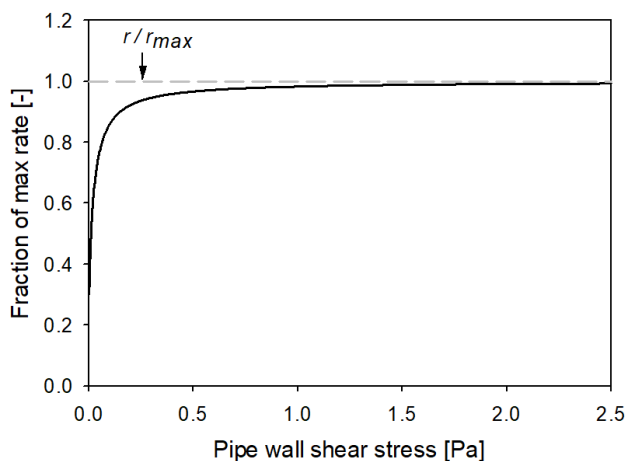


Figure 119. Relation between the maximum sulfide formation rate ( $r_{max}$ ) and the actual rate ( $r$ ). The parameters used to plot the figure were  $k_{T0} = 0.3$  and  $K_T = 0.025$

#### 9.4.7 Sulfide oxidation in the wastewater

Sulfide is oxidized aerobically in the bulk water and biofilms of sewers when there is oxygen present. The oxidation occurs both biologically and chemically. The details of the processes are given in the file *WATS matrix*, which is an addendum to this manual. The parameters for these processes are entered in the grid shown in Figure 119. Sulfide can also be oxidized anoxically, the parameters for these processes are entered in the grid shown in Figure 120.

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default CDD Compounds pH_buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Rate constant for chemical oxidation of H2S (oxidation with O2)	gH2S-S/(m3 d)	0.960	0.240	0.010	100.000	Fixed
Rate constant for chemical oxidation of HS- (oxidation with O2)	gHS-S/(m3 d)	12.000	2.400	0.100	100.000	Fixed
Rate constant for biological oxidation of sulfide	gH2S-S/(m3 d)	12.000	2.400	0.100	100.000	Fixed
pH optimum for heterotrophic and autotrophic processes	-	7.5	1.0	6.5	8.5	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - bulk water (ox with O2)	gS/gO2	0.900	0.100	0.500	2.000	Fixed
Stoichiometric reaction coefficient of biological sulfide oxidation - bulk water (ox with O2)	gS/gO2	2.000	0.100	0.500	2.000	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - biofilm (ox with O2)	gS/gO2	2.000	0.100	0.500	2.000	Fixed
Sulfide biofilm biological oxidation rate (ox with O2)	gS/(m2 d)	2.400	0.240	0.240	48.000	Fixed
Sulfide bulk water chemical oxidation order with respect to sulfide (ox with O2)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water chemical oxidation order with respect to oxygen (ox with O2)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to sulfide (ox with O2)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to oxygen (ox with O2)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to sulfide (ox with O2)	-	0.500	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to oxygen (ox with O2)	-	0.500	0.100	0.000	1.000	Fixed
Parameter accounting for the width of the biological sulfide oxidation pH dependency	-	25.00	5.00	10.00	100.00	Fixed
Arrhenius constant for the chemical oxidation of sulfide	-	1.070	0.010	1.000	1.150	Fixed
Arrhenius constant for the biological oxidation of sulfide in the bulk water	-	1.070	0.010	1.000	1.100	Fixed

Figure 120. Aerobic sulfide oxidation

Model parameters						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl- Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Rate constant for chemical oxidation of H2S (oxidation with NO2+NO3)	gH2S-S/(m3 d)	0.000200	0.000100	0.000000	0.010000	Fixed
Rate constant for chemical oxidation of HS- (oxidation with NO2+NO3)	gHS-S/(m3 d)	0.050000	0.010000	0.001000	1.000000	Fixed
Rate constant for biological oxidation of sulfide (oxidation with NO2+NO3)	gH2S-S/(m3 d)	0.500	0.100	0.010	10.000	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - bulk water (ox with NO2+NO3)	gS/gNO	2.574	0.286	1.430	5.720	Fixed
Stoichiometric reaction coefficient of biological sulfide oxidation - bulk water (ox with NO2+NO3)	gS/gNO	5.720	0.286	1.430	5.720	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - biofilm (ox with NO2+NO3)	gS/gNO	5.720	0.286	1.430	5.720	Fixed
Sulfide biofilm biological oxidation rate (ox with NO2+NO3)	gS/(m2 d)	0.500	0.050	0.005	5.000	Fixed
Sulfide bulk water chemical oxidation order with respect to sulfide (ox with NO2+NO3)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water chemical oxidation order with respect to NO2+NO3 (ox with NO2+NO3)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to sulfide (ox with NO2+NO3)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to NO2+NO3 (ox with NO2+NO3)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to sulfide (ox with NO2+NO3)	-	0.500	0.100	0.000	1.000	Fixed

Figure 121. Anoxic sulfide oxidation

#### 9.4.8 Fermentation

Fermentation occurs during anaerobic conditions. It takes place in the biofilm and the bulk water. Mega-WATS models fermentation of  $S_F$  (fermentable substrates, section 9.1.2) and  $X_{Sf}$  (fast hydrolysable substrate, section 9.1.2). In the biofilm it is a half order rate process, while it is a biomass dependent process in the bulk water, with the fermenting biomass ( $X_{Hferm}$ , section 9.1.1) determining the rate. The parameters for these processes are entered in the grid shown in Figure 121.

Model parameters						
Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl- Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Anaerobic hydrolysis efficiency constant ( $\eta_{h,anaerobic}$ )	-	0.300	0.050	0.100	0.600	Fixed
Rate constant for biofilm fermentation at 20°C ( $q_{FermF}$ )	(mgCOD/(m2h))^0.5	15.0	4.5	2.5	250.0	Fixed
Fraction of fermentation rate when using $X_{Sf}$	-	0.1	0.0	0.0	1.0	Fixed
Rate constant for bulk water fermentation at 20°C ( $q_{FermW}$ )	1/d	1.500	0.450	1.000	10.000	Fixed
Saturation constant for bulk water fermentation ( $K_{FermW}$ )	gCOD/m3	0.500	0.150	0.010	10.000	Fixed
Yield constant for fermenter growth on SF	(gCOD/gCOD)	0.080	0.024	0.008	0.400	
Decay rate constant for fermenters ( $b_{Xferm}$ )	d-1	2.00	0.20	0.02	20.00	Fixed
Methyl mercaptan formation rate as fraction of the fermentation rate ( $q_{MM}$ )	1/d	0.0020	0.0010	0.0002	0.0200	Fixed
Methyl mercaptan oxidation rate as fraction of the sum of all oxidation rates ( $o_{MM}$ )	1/d	0.2000	0.1000	0.0100	0.6000	Fixed

Figure 122. Fermentation, anaerobic hydrolysis, and methyl mercaptan formation



#### 9.4.9 Methyl mercaptan formation and oxidation

Methyl mercaptan, or methanethiol as it is also called, is formed by fermentative processes during anaerobic conditions. The process is poorly understood, and it is hence assumed a fraction of the processes causing fermentation products ( $S_A$ ). The same goes for its oxidation, which is similarly modeled as a fraction of the overall oxidation of fermentation products (Figure 121).

#### 9.4.10 Methane formation

Methane formation is fully implemented in Mega-WATS. However, the possibility to use this function is only made available upon request, as this aspect should not be used without thorough model calibration.

#### 9.4.11 Anoxic processes, denitrification

Anoxic processes, also called denitrification, are simulated as a two-stage process where nitrate ( $\text{NO}_3^-$ ) is reduced to nitrite ( $\text{NO}_2^-$ ), which then is reduced to free nitrogen ( $\text{N}_2$ ). Mega-WATS hence includes nitrate, nitrite, and free nitrogen as state variables. Of these, the user only sees nitrate in the visualizations.

The parameters for anoxic conditions are set on the pages *Bulk ww anoxic* (Figure 122) and *Biofilm anoxic* (Figure 123).

Model parameters						
Default CDD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Maximum growth rate of het. biomass utilizing $\text{NO}_3$ at 20°C (my)	1/d	1.00	0.50	0.20	6.00	Fixed
Maximum growth rate of het. biomass utilizing $\text{NO}_2$ in the presence of $\text{NO}_3$ at 20°C (my)	1/d	1.50	0.50	0.20	6.00	Fixed
Maximum growth rate of het. biomass utilizing $\text{NO}_3$ in the absence of $\text{NO}_3$ at 20°C (my)	1/d	1.50	0.50	0.20	6.00	Fixed
Yield constant for bulk water anoxic heterotrophic biomass (YHwNO)	mol e-eq/mol e-eq	0.450	0.050	0.100	0.600	Fixed
Saturation constant for het. growth on nitrate (KNO3)	gN/m3	0.600	0.200	0.200	10.000	Fixed
Saturation constant for het. growth on nitrite (KNO2)	gN/m3	0.300	0.100	0.100	10.000	Fixed
Maintenance rate during $\text{NO}_3$ respiration	1/d	0.083	0.050	0.010	0.800	Fixed
Maintenance rate during $\text{NO}_2$ respiration in the presence of $\text{NO}_3$	1/d	0.125	0.050	0.010	0.800	Fixed
Maintenance rate during $\text{NO}_2$ respiration in the absence of $\text{NO}_3$	1/d	0.125	0.050	0.010	0.800	Fixed
Relative hydrolysis under anoxic conditions compared to oxic conditions (fryNOh)	-	0.60	0.10	0.40	1.00	Fixed
Saturation constant under anoxic conditions (KNO)	gNO/m3	0.500	0.100	0.100	2.000	Fixed

Figure 123. Anoxic bulk water process parameters

Model parameters						
Default COD   Compounds   pH, buffers   General   Bulk ww aerobic   Biofilm aerobic   Sulfide form, biofilm   Sulfide form, ww   Sulfide ox, aerobic   Sulfide ox, anoxic   Sulfide ox, gas Anaerobic ferm.   Bulk ww anoxic   Biofilm anoxic   H2O2 Dosing   HOCI Dosing   Iron dosing   FeS ox.   Drops   Turbulences   Structures   Tracer						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
½ order rate constant for biofilm, NO3 reduction (k½NO3)	(gN/m)½ 1/d	1.000	0.500	0.200	10.000	Fixed
½ order rate constant for biofilm, NO2 reduction in the presence of NO3(k½NO2I)	(gN/m)½ 1/d	1.500	0.500	0.300	10.000	Fixed
½ order rate constant for biofilm, NO2 reduction in the absence of NO3(k½NO2II)	(gN/m)½ 1/d	1.500	0.500	0.300	10.000	Fixed
Yield constant for biofilm biomass, anoxic conditions (YHfNO)	mol e-eq/mol e-eq	0.370	0.050	0.200	0.600	Fixed

Figure 124. Anoxic biofilm process parameters

#### 9.4.12 Nitrification

For reasons of completeness, Mega-WATS allows nitrification to occur under conditions where degradable COD becomes depleted. However, it does not contain any ammonia oxidizing biomass as no such biomass can exist under typical sewer conditions. Here the autotrophic ammonia oxidizers grow much slower than the heterotrophs and hence lose the competition for oxygen in the biofilm.

#### 9.4.13 Concrete corrosion and oxidation of H<sub>2</sub>S on moist surfaces

Once H<sub>2</sub>S is present in the sewer air of a gravity pipe, it can be lost/gained by several processes.

##### 9.4.13.1 Exchange with dissolved sulfide in the wastewater

If the concentration in the air is below the equilibrium defined by Henry's law, H<sub>2</sub>S will transfer from the water to the air. If it is above the equilibrium, H<sub>2</sub>S will be transferred from the air to the water. In a gently flowing gravity main this mass transfer across the liquid-gas boundary is slow compared to the rate by which H<sub>2</sub>S is absorbed by corroding concrete. This leads to gas phase concentrations often being significantly below the equilibrium defined by Henry's law.

In a long gravity main, the final concentration in the sewer air will be defined by the following balance:

$$r_{H_2S\text{releaseWater}} = r_{H_2S\text{uptakeConcrete}}$$

where  $r_{H_2S\text{releaseWater}}$  is the rate by which H<sub>2</sub>S is released from the flowing water of a gravity main and into the sewer air.

where  $r_{H_2S\text{uptakeConcrete}}$  is the rate by which H<sub>2</sub>S is taken up by the corroding concrete.

Both rates depend on the concentration of H<sub>2</sub>S in the sewer air.

$r_{H_2S\text{releaseWater}}$  decreases the more H<sub>2</sub>S there is in the sewer air. The closer the H<sub>2</sub>S concentration in the air gets to the theoretical equilibrium concentration, the slower the process (when they are equal, the transfer rate is zero). See also section 9.5.1.1 on liquid-gas mass transfer in partly filled pipes.

$r_{H_2S\text{uptakeConcrete}}$  increases with increasing H<sub>2</sub>S gas concentration.

The overall result is that sewer air concentrations typically are much below the theoretical gas phase concentration (often in the range of a few percent of what they could be).

Another very important aspect of this balance is that one absolutely cannot predict corrosion rates from gas phase concentrations. This has been done in several cases; however, it is a logical fallacy as the corrosion is controlled by the mass transfer of H<sub>2</sub>S onto the sewer surface as described above. This is best illustrated by an example of corrosion in a long sewer pipe:

The corrosion rate depends on how much H<sub>2</sub>S is oxidized to sulfuric acid per unit of time. This will depend on how active the microorganisms are and on how fast the H<sub>2</sub>S is absorbed by the moist concrete surface. Speculating that one forces the H<sub>2</sub>S-gas concentration in a sewer to be held at a fixed concentration (e.g., by supplying H<sub>2</sub>S gas from a gas flask), this would lead to higher H<sub>2</sub>S-gas concentrations causing more corrosion (as both the biological activity and the adsorption to the concrete surface is faster at higher concentrations). And here is where the logical fallacy comes in. While the H<sub>2</sub>S-gas can be kept at a fixed concentration in a test chamber in the lab, this is not possible in a sewer, as the H<sub>2</sub>S gas comes from being stripped from the water to the air.

The limiting factor for the corrosion rate becomes the rate by which H<sub>2</sub>S can be released from the water to the sewer air. This rate is governed by the mass transfer equation:

$$\frac{dS_{H_2S}}{dt} = \alpha K_L a (\beta S_{H_2S} - H_{H_2S} p_{H_2Sg})$$

Where  $S_{H_2S}$  is the water phase H<sub>2</sub>S concentration,  $\alpha$  and  $\beta$  are constants which typically are set to 1,  $K_L a$  is the mass transfer coefficient,  $H_{H_2S}$  is the henry's constant, and  $p_{H_2Sg}$  is the partial pressure of H<sub>2</sub>S in the sewer air (Section 9.5.1).

Assume now that the microorganisms are highly active and the H<sub>2</sub>S is absorbed very fast by the moist concrete surface. This leads to the resulting H<sub>2</sub>S-gas concentration being low, as the released H<sub>2</sub>S is taken up fast. The lowering of the H<sub>2</sub>S-gas concentration will furthermore result in a high release rate as determined by the mass transfer equation, as  $S_{H_2S}$  is constant while  $p_{H_2Sg}$  decreases, leading to the number in the bracket becoming larger.

Assume now the opposite situation, where the microorganisms have low activity and the H<sub>2</sub>S is absorbed slowly by the moist concrete surface. This will lead to higher H<sub>2</sub>S gas concentrations and slower H<sub>2</sub>S-gas release.

In other words, a high H<sub>2</sub>S-gas concentration in the sewer air is not indicative of the corrosion rate but is the result of balancing the release rate and the uptake rate. Assuming the only variable is the activity of the microorganisms and H<sub>2</sub>S absorption rate, and all else being equal, this means that a higher H<sub>2</sub>S gas concentration means a lower corrosion rate, i.e., quite counter-intuitive. This phenomenon is also observed in real life: When measuring H<sub>2</sub>S-gas in corroding concrete sewer, one often finds quite low concentrations. If the sewer then is lined, the H<sub>2</sub>S-gas concentrations jumps up because the plastic surface is not able to take up nearly as much H<sub>2</sub>S as the concrete surface was.

The above-described balance is also what already was described by USEPA (1974), and it was the H<sub>2</sub>S flux from the water to the air which already back then was used to predict corrosion rates. The only place where one can assume correlation between H<sub>2</sub>S gas concentrations and corrosion rates (with some realism but still not process-wise correctly) is close to hotspots like drop structures, where the above stated equilibrium has not yet been established.

#### 9.4.13.2 The rate by which H<sub>2</sub>S is captured by the corroding concrete surface

H<sub>2</sub>S in the sewer air is transferred to the corroding concrete by turbulent movements in the air. How this transport happens will depend on local air flow patterns in the pipe. For large pipes with slow flowing air, this process is not well understood. For small pipes there is experimental evidence on how the H<sub>2</sub>S mass transfer occurs. Several studies were done on this, where a pilot setup was used, consisting of several 200 mm diameter concrete pipes, holding wastewater, having forced air circulation, and into which H<sub>2</sub>S gas was injected. This simulated the intermittent discharge from a force main into a gravity sewer. The speed of H<sub>2</sub>S decline after injections was then monitored. The first study on this was Vollertsen et al. (2008), showing that the change in H<sub>2</sub>S gas could be described as:

$$\frac{dp_{H_2S}}{dt} = k_p p_{H_2S}^n$$

The median value for the exponent  $n$  was determined to 0.54. For plastic pipes it was 0.61.

The second study was Nielsen et al. (2008), who compared H<sub>2</sub>S oxidation rates by concrete to those of plastic pipes, finding that oxidation on concrete pipes was roughly 30-50 times faster on concrete than on plastics. This means that the equilibrium between  $r_{H_2S\text{releaseWater}}$  and  $r_{H_2S\text{uptakeConcrete}}$  will establish itself at a higher gas phase concentration. In other words, sewer air H<sub>2</sub>S gas concentrations are heavily affected by pipe material (corrodible versus non-corrodible). That publication also discusses what happens if the layer of corrosion material that establishes itself on concrete becomes intermittently scoured off.

In a study by Nielsen et al. (2012), the impact of air velocity (Reynolds number) on the corrosion rate was addressed. It was studied in the previously used 200 mm concrete pipe setup. The main finding was that the uptake of H<sub>2</sub>S gas depended on the Reynolds number of the air flow.

$$\frac{dp_{H_2S}}{dt} = k_p \text{Re}^m p_{H_2S}^n$$

The exponent  $m$  was determined to 0.65 while the exponent  $n$  was determined to 0.8.  $k_p$  ranged from 0.010 to 0.068, with a median value of 0.047.

An issue with the above equation is that when the Reynolds number gets small, the uptake by the concrete gets small, ultimately close to zero (0.015 in the equation below) when the air stands still. To account for this, Mega-WATS applies:

$$\frac{dp_{H_2S}}{dt} = (k_p \text{Re}^m + 0.015) p_{H_2S}^n$$

Where the constant 0.015 is somewhat arbitrary and only intended ensure some corrosion in pipes and chambers where the air stands still.

#### 9.4.13.3 Average versus peak corrosion rates

The simulated concrete corrosion is an average rate over the perimeter of the pipe. Local corrosion rates will be higher or lower than the simulated value. It is for example common, that crown corrosion is more severe than corrosion on the vertical part of the pipe walls. How much can be difficult to predict, but peak corrosion can readily be more than twice as severe as the average.

Predicting failure, a factor should hence be applied on the average corrosion rate. Albeit it remains uncertain how large such factor should be, it seems likely it is in the range of 1.5 – 2.5. See also Section 7.2.

#### 9.4.13.4 How captured H<sub>2</sub>S gas ends up corroding the concrete

Once H<sub>2</sub>S is absorbed on the concrete surface, it is oxidized by oxygen. Already USEPA (1974) identified the fundamental equation for the corrosion rate:

$$r_{corr} = k \frac{100 F}{32 A}$$

Where

$F$  is the rate of hydrogen sulfide absorption in the moisture at the concrete surface (g H<sub>2</sub>S-S m<sup>-2</sup> h<sup>-1</sup>).

$A$  is the alkalinity of the concrete material in units of g CaCO<sub>3</sub> per g concrete material.

$k$  is a correction factor considering that not all absorbed H<sub>2</sub>S results in corrosion.

It was already back then assumed that for systems where the H<sub>2</sub>S absorption rate is low,  $k$  approaches 1, while at increasing values of  $F$ ,  $k$  may decrease to about 0.3–0.4. This was believed to be because acid was lost by droplets falling off the surfaces and into the water. Later it was shown that this is not how it happens, but that this observed phenomenon is caused by the H<sub>2</sub>S first being converted to elemental sulfur, and then to sulfuric acid, which then attacks the concrete. At high H<sub>2</sub>S absorption rates, the first step is favored, causing an accumulation of elemental sulfur. This sulfur then crystalizes into a form which is only slowly accessible by bacteria. More of this can be read in the PhD work of Henriette Jensen et al., Aalborg, Denmark.

The correction factor  $k$  was further studied by Nielsen et al. (2014). They partly confirmed in pilot scale what was already shown at lab scale by H. Jensen, and partly were able to quantify the value of  $k$ . They did this in the same setup as previously discussed. They found that an assumption of a fixed value of  $k$  was not supportable, and that the value indeed depended on the surface loading rate, as was already reported by USEPA (1974). However, Nielsen et al. (2014) showed that the mechanisms were more complex than such: When a concrete surface is subject to H<sub>2</sub>S, it converts some to elemental sulfur which accumulates and some to sulfuric acid which attacks the concrete. They observed that the value  $k$  was roughly between 0.9 and 0.3 for the loading range they applied. However, they also saw that when turning off the H<sub>2</sub>S exposure, corrosion continued due to a slower oxidation of the stored elemental sulfur, leading to higher  $k$  values.

The above observed phenomena make the prediction of corrosion somewhat difficult, as one must take many aspects into account to reproduce the true behavior of a system. For example, if a pipe becomes submerged, washing off the corrosion products, hereby stripping the storage of elemental sulfur. In any case, however, there must be some relationship between surface loading (how much H<sub>2</sub>S the concrete surface experiences over time) and the efficiency in converting this to corrosion attack. The higher the loading, the lower the efficiency. The exact function, and the exact values hereof is though still poorly known.

To implement this in Mega-WATS, the following equation is used to fit the data observed by Nielsen et al. (2014):

$$k_{corr} = a_1 e^{(-b_1 x)} + a_2 e^{(-b_2 x)} + a_3$$

and if  $k_{corr} > 1$  then  $k_{corr} = 1$

where  $x$  is  $r_{H_2S \text{ uptake Concrete}} / 24$

$a_1, a_2, a_3, b_1, b_2$  are constants used to fit the field observations of concrete corrosion penetration depth.

There is no guarantee that studies conducted in pilot scale can be transferred to full scale on a one-to-one basis. But if there are no systematic full-scale datasets casting light over the phenomena, this is the best there is.

Due to this uncertainty, users might choose to change some parameters. All process parameters can be adjusted by the user, but when doing so, the user must understand the processes behind.

One aspect to consider is that the surface specific uptake rates measured in the pilot, and which are used as default in Mega-WATS are probably fine for small bore pipes but probably too high for large bore pipes. They should hence be calibrated based on measurements.

## 9.5 Physical processes

### 9.5.1 Liquid-gas mass transfer

The mass transfer between liquid and gas is handled for three fundamentally different situations:

- The flowing sewer where gas slowly is released from the liquid to the sewer air
- Sewer drops (waterfalls) where a high release occurs in one spot
- Sharp bends in the sewer inducing minor hydraulic losses to the flow

For all cases, the two-film theory is applied with oxygen as the tracer gas. This means that all resistance to mass transfer is assumed to be in the liquid film and none in the gas film – a good assumption for the slightly soluble gases of interest. The transfer of relatively insoluble gases other than oxygen is analogous to oxygen transfer. The analogy is established via the diffusivity of the substances in the water. For substances where part or most of the resistance lies in the gas film, empirical data on how this resistance can be linked to that of the water is used. For details see Matias et al. (2018).

It is hence paramount to have good empirical equations which can simulate the three situations of mass transfer.

#### 9.5.1.1 Partly filled pipe

This process is often called reaeration and occurs due to the turbulence caused by the water flowing in a partly filled pipe. The concept originates from open channel oxygen balance models, such as the Streeter–Phelps equation from the 1920s. Numerous studies have since then attempted to improve the prediction of oxygen mass transfer across the gas-liquid boundary of water flowing with a free surface. The general agreement is that this process shall be described by a factor multiplied by the oxygen deficit, i.e., how far the flowing water is from equilibrium with the ambient air:

$$K_L a_{O_2} \alpha_{rea} (\beta_{rea} S_{O_{sat}} - S_O)$$

The reaeration occurs over the surface area and the oxygen is mixed into the water volume. Hence, a lumped constant termed  $K_L a$  is defined, where the term  $K_L$  stands for flux through the water surface and the term  $a$  stands for the average water depth of the cross-section. The terms  $\alpha_{rea}$  and  $\beta_{rea}$  are correction factors between pure water and wastewater (they can be set as described in section 9.3).

For a partly filled sewer, Mega-WATS uses the following equation to determine  $K_L a$  for oxygen:

$$K_L a_{O_2} = 24 \cdot 0.86(1 + 0.20F^2)(su)^{\frac{3}{8}} d_m^{-1} \alpha_r^{T-20}$$

Where  $F$  is the Froude number of the flow,  $s$  the slope of the energy line,  $u$  the velocity of the water,  $d_m$  the mean depth,  $\alpha_r$  a temperature correction constant, and  $T$  the temperature.

#### 9.5.1.2 Drop structures

Drop structures are simulated as the drop occurring on the upstream pipe (Figure 124). The air with which the water interacts – either by release or uptake – comes from the upstream pipe. In case the upstream pipe has no air (e.g., if it is a force main), the air comes from the ambient atmosphere. The water and the air after the drop are then mixed into the water and air from other connections, including air intake from the ambient atmosphere at the manhole.

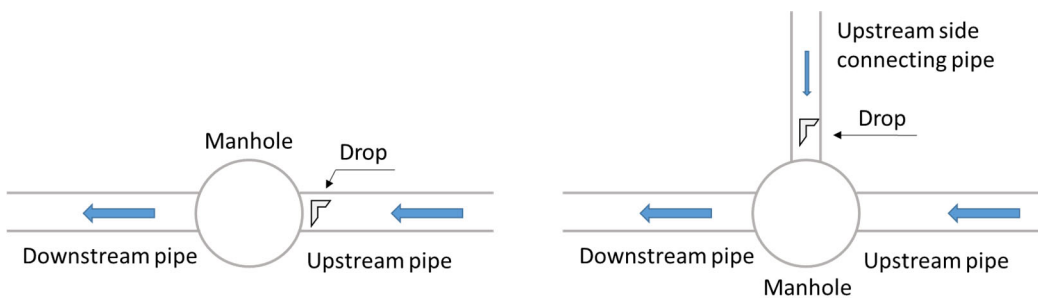


Figure 125. Simulated location of drops within the sewer network

For a drop structure,  $K_L a_{O_2}$  is calculated from an empirical equation for the oxygen deficit ratio:

$$r_O = \frac{S_{OS} - S_{Oup}}{S_{OS} - S_{Odw}}$$

Where	$r_O$	oxygen deficit ratio [-]
	$S_{OS}$	oxygen saturation concentration [mg/L]
	$S_{Oup}$	oxygen saturation upstream of the drop [mg/L]
	$S_{Odw}$	oxygen saturation downstream of the drop [mg/L]

The mass transfer of other volatile substances is determined based on the two-film theory.

Drop structures are described by an equation considering the drop height, water flow, and the tailwater depth into which the water plunges. The equation for the oxygen deficit ratio is:

$$\ln r_O = c_1 H_{drop}^{c_2} Q_{drop}^{c_3} h_{tail}^{c_4}$$

Where	$c_1-c_4$	constants ( $c_1, c_2, c_4$ are positive, $c_3$ is negative)
	$H_{drop}$	drop height from water surface to water surface
	$Q_{drop}$	flow over the drop
	$h_{tail}$	tail water depth (downstream water depth)

The oxygen deficit ratio is converted into a  $K_L a_{O_2}$  value as  $K_L a_{O_2} \frac{V}{Q} = -\ln(r_C)$ , which then can be used to deduct the  $K_L a$  value of other volatile substances.



Mega-WATS allows four different drop types to be configured by the user (Figure 125): Fall, Plunge, Vortex, and Helix. Each is described by the same equation but using different parameters. The type of drop is set in the network file, see section 4.2.1.14.

Model parameters

Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer

The drop parameters:  $\exp(a \cdot H_{drop} \cdot a_{Drop} \cdot Q^a \cdot a_{Flow} \cdot H_{tail} \cdot a_{Tail})$

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Minimum drop height	m	0.025	0.006	0.003	0.250	Fixed
Type Fall: a (a factor)	-	0.200	0.050	0.020	2.000	Fixed
Type Fall: aDrop (the exponent for Hdrop)	-	0.750	0.188	0.075	7.500	Fixed
Type Fall: aFlow (the exponent for Q)	-	-0.200	-0.050	-0.020	-2.000	Fixed
Type Fall: aTail (the exponent for Htail)	-	0.100	0.025	0.010	1.000	Fixed
Type Plunge: a (a factor)	-	0.200	0.050	0.020	2.000	Fixed
Type Plunge: aDrop (the exponent for Hdrop)	-	0.750	0.188	0.075	7.500	Fixed
Type Plunge: aFlow (the exponent for Q)	-	-0.200	-0.050	-0.020	-2.000	Fixed
Type Plunge: aTail (the exponent for Htail)	-	0.100	0.025	0.010	1.000	Fixed
Type Vortex: a (a factor)	-	0.200	0.050	0.020	2.000	Fixed
Type Vortex: aDrop (the exponent for Hdrop)	-	0.750	0.188	0.075	7.500	Fixed
Type Vortex: aFlow (the exponent for Q)	-	-0.200	-0.050	-0.020	-2.000	Fixed
Type Vortex: aTail (the exponent for Htail)	-	0.100	0.025	0.010	1.000	Fixed
Type Helix: a (a factor)	-	0.200	0.050	0.020	2.000	Fixed
Type Helix: aDrop (the exponent for Hdrop)	-	0.750	0.188	0.075	7.500	Fixed
Type Helix: aFlow (the exponent for Q)	-	-0.200	-0.050	-0.020	-2.000	Fixed
Type Helix: aTail (the exponent for Htail)	-	0.100	0.025	0.010	1.000	Fixed

Figure 126. Setup of drop structures

### 9.5.1.3 Special considerations for gases with low Henry's constant

Gases with low Henry's constant must be modelled at a smaller space step than other gases as results otherwise are numerically unstable. One example is ammonia, which must be simulated at space steps as low as 0.01 – 0.1 m instead of the 1 m which is the default setting of Mega-WATS.

### 9.5.1.4 Minor losses

Hydraulic minor losses are calculated like for drop structures, and so they are calculated assuming the drop height  $H_{drop}$  equals the minor energy loss in units of meters water column. Minor losses are restricted to occur under certain conditions, namely if the angle between two pipes exceeds a certain value, and if the flow velocity exceeds a certain value (Figure 126).

Model parameters

Default COD Compounds pH, buffers General Bulk ww aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. ww Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas Anaerobic ferm. Bulk ww anoxic Biofilm anoxic H2O2 Dosing HOCl-Dosing Iron dosing FeS ox. Drops Turbulences Structures Tracer

Reaeration is also calculated at bents in the pipe under the following conditions  
They are calculated assuming that the minor loss at the bent equals a drop height

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Minimum angle between pipes (radians)	-	0.1750	0.0437	0.0175	1.7500	Fixed
Minimum flow velocity (m/s)	-	0.500000	0.125000	0.050000	5.000000	Fixed

Figure 127. Minor loss parameters

### 9.5.2 Hydraulic jumps

Hydraulic jumps occur in principle when flow goes from critical (Froude number ( $Fr$ ) is  $>1$ ) to sub-critical ( $Fr$  is  $<1$ ). Hydraulic jumps are very difficult to predict, but hydraulic experience says that  $Fr$  below 1.7, the jump is very weak and does not lead to a disruption of the water surface. While when  $Fr$  is above 9.0, the shape of the jump does not change with increasing Froude number.

Froude number	Ratio of height after to height before jump	Description of jump	Energy dissipation
$\leq 1.0$	1.0	No jump	none
<b>1.0–1.7</b>	1.0–2.0	Standing or undulating wave	$< 5\%$
<b>1.7–2.5</b>	2.0–3.1	Weak jump (series of small rollers)	$5\% - 15\%$
<b>2.5–4.5</b>	3.1–5.9	Oscillating jump	$15\% - 45\%$
<b>4.5–9.0</b>	5.9–12.0	Stable clearly defined well-balanced jump	$45\% - 70\%$
<b><math>&gt; 9.0</math></b>	$> 12.0$	Clearly defined, turbulent, strong jump	$70\% - 85\%$

Turbulence at a hydraulic jump leads to an increased mass transfer rate across the gas-liquid boundary. However, how much it increases is not well studied under sewer conditions. From other systems it is known that the gas transfer rate can be predicted from the energy loss, which again is related to the change in water depth upstream and downstream of the jump.

A hydraulic jump is simulated as if it occurs on the upstream pipe (Figure 127). The air with which the water interacts – either by release or uptake – comes from the upstream pipe. The water and the air after the drop are then mixed into the water and air from other connections, including air intake from the ambient atmosphere at the manhole.

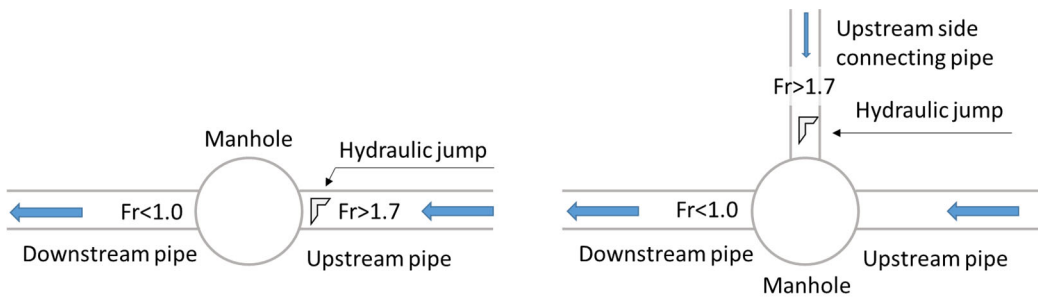


Figure 128. Simulated location of hydraulic jumps within the sewer network

In Mega-WATS, the gas-liquid mass transfer rate is calculated as the reaeration rate of the upstream pipe multiplied by a factor depending on the Froude number in the upstream pipe and on the length of the jump. The latter is calculated as  $L_{jump} = (y_{dw} - y_{up})(7.6 - 0.1Fr)$  when the drop occurs inside a pipe. This can occur when backwater stems up in a pipe (mainstream or side connection) and causes the jump. If the drop occurs at a manhole, the downstream water depth is assumed twice the upstream depth.

The parameters related to the Froude number can be set in the turbulence page of the parameter input form (Figure 129).

Model parameters						
Default COD   Compounds   pH, buffers   General   Bulk ww aerobic   Biofilm aerobic   Sulfide form. biofilm   Sulfide form. ww   Sulfide ox. aerobic   Sulfide ox. anoxic   Sulfide ox. gas Anaerobic ferm.   Bulk ww anoxic   Biofilm anoxic   H2O2 Dosing   HOCl Dosing   Iron dosing   FeS ox.   Drops <b>Turbulences</b> Structures   Tracer						
Below Fr=1.7 no hydraulic jump. Between the values below: Linear interpolation between KLa-factors. Above Fr=9.0 the KLa-factor is constant						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Factor to multiply KLa when hydraulic jump Froude Number = 1.7 (weak jump)	-	5.00	1.25	0.50	50.00	Fixed
Factor to multiply KLa when hydraulic jump Froude Number = 2.5 (oscillating jump)	-	8.00	2.00	0.80	80.00	Fixed
Factor to multiply KLa when hydraulic jump Froude Number = 4.5 (stable clearly defined balanced jump)	-	15.00	3.75	1.50	150.00	Fixed
Factor to multiply KLa when hydraulic jump Froude Number = 9.0 (clearly defined, turbulent, strong jump)	-	25.00	6.25	2.50	250.00	Fixed

Figure 129. Parameters for scaling reaeration by hydraulic jump Froude number

## 9.6 Default turbulence at force main discharge nodes

Force main discharges are typically (but not always) turbulent. This can be reflected by assigning a drop structure to the turbulent discharge node, i.e., artificially creating a height difference between the force main and the receiving pipe.

To avoid doing this for all force main discharges, one can set the default turbulence as an equivalent drop height, calculated as described in section 9.5.1.2.

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Default drop height assumed at force main discharge to simulate turbulence (drop type = Fall)	m	0.50	0.13	0.05	5.00	Fixed
Default configuration, force main discharges						
<input checked="" type="radio"/> Free fall <input type="radio"/> Plunge <input type="radio"/> Vortex <input type="radio"/> Helix						

Figure 130. Equivalent drop height for default force main discharges

## 9.7 Structures and chambers

Mega-WATS can include chambers where the water and air is simulated as completely mixed. Default values for chambers is given on the *Structures* page (Figure 130). The water depth and the  $K_La$  value can also be set individually in the network file (Section 4.2.1.5.4).

The correction factor for  $H_2S$  formation considers that sediments in chambers may cause increased formation rates. The factor on air velocity affects the corrosion of concrete chambers.

Model parameters

Default COD   Compounds   pH, buffers   General   Bulk ww aerobic   Biofilm aerobic   Sulfide form biofilm   Sulfide form. ww + gen.   Sulfide ox. aerobic   Sulfide ox. anoxic   Sulfide ox. gas  
 Fermentation   Bulk ww anoxic   Biofilm anoxic   H2O2 Dosing   HOCl Dosing   Iron dosing   FeS ox.   Drops   Turbulences   Structures   Tracers   CH4 biofilm   CH4 bulk water

Parameters for nodes and chambers, such as pump stations, and for backwater created by weirs and diurnal flow restrictions

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Correction factor for $H_2S$ -formation rate in nodes and chambers	-	1.00	0.25	0.10	10.00	Fixed
Correction factor for $CH_4$ -formation rate in nodes and chambers	-	1.00	0.25	0.10	10.00	Fixed
Default water depths in chambers	m	0.50	0.13	0.05	5.00	Fixed
Default $K_La$ in chambers	1/d	0.00	0.00	0.00	0.00	Fixed
Correction factor for $H_2S$ -formation rate in backwater pipes when restricting the flow diurnally	-	1.00	0.25	0.10	10.00	Fixed
Correction factor for $CH_4$ -formation rate in backwater pipes when restricting the flow diurnally	-	1.00	0.25	0.10	10.00	Fixed
Factor increasing air velocity in nodes and chambers (increases corrosion)	-	1.0	0.3	0.1	10.0	Fixed

Figure 131. Parameters for chambers (completely mixed reactors)

## 10 Chemical treatment of odor and corrosion

Adding chemicals to wastewater can be done through a dosing file loaded as part of the project setup or by adding chemicals via the user interface after the model has been run.

### 10.1 The chemicals treatment mechanisms

Mega-WATS includes common chemicals used for dosing:

- Ferrous iron, Fe(II)
- Ferric iron, Fe(III)
- Nitrate (measured as NO<sub>3</sub>-N)
- Oxygen
- Hydrogen peroxide (measured as H<sub>2</sub>O<sub>2</sub> mass)
- Hypochlorite (measured as OCl mass)
- Base (measured in moles)
- Magnesium hydroxide (measured in Mg mass)

#### 10.1.1 Ferrous and ferric iron

Parameters controlling the chemistry of iron are set in the simulation parameters menu (Figure 131). *Input* → *Set model parameters* → *Iron dosing*

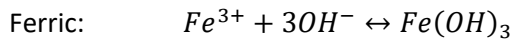
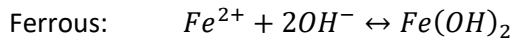
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Reduction factor for acid formation when dosing ferrous (FeII) compared to theoretical value	-	0.80	0.10	0.10	1.00	Fixed
Reduction factor for acid formation when dosing ferric (FeIII) compared to theoretical value	-	0.80	0.10	0.10	1.00	Fixed
The min ratio Psi in: $R_{Fe:S} = \Psi_{Si+a}(pK-pH)^n$ (Molar Ratio of conversion)	-	1.15	0.29	0.11	11.50	Fixed
The factor a in: $R_{Fe:S} = \Psi_{Si+a}(pK-pH)^n$ (Molar Ratio of conversion)	-	0.50	0.13	0.05	5.00	Fixed
The constant pK in: $R_{Fe:S} = \Psi_{Si+a}(pK-pH)^n$ (Molar Ratio of conversion)	-	8.0	2.0	0.8	80.0	Fixed
The exponent n in: $R_{Fe:S} = \Psi_{Si+a}(pK-pH)^n$ (Molar Ratio of conversion)	-	2.0	0.5	0.2	20.0	Fixed
K <sub>rm</sub> at pH 6.5 [mol/mol]	-	0.0500	0.0125	0.0050	0.5000	Fixed
K <sub>rm</sub> at pH 8.5 [mol/mol]	-	0.00500	0.00125	0.00050	0.05000	Fixed
Offset of R <sub>m</sub>	-	0.01000	0.00250	0.00100	0.10000	Fixed
The constant k in: $k \cdot [Stot]^n \cdot [FeOH2]^m$ (FeS precipitation)	-	450	113	45	4500	Fixed
The exponent n in: $k \cdot [Stot]^n \cdot [FeOH2]^m$ (FeS precipitation)	-	1.00	0.25	0.10	10.00	Fixed
The exponent m in: $k \cdot [Stot]^n \cdot [FeOH2]^m$ (FeS precipitation)	-	1.00	0.25	0.10	10.00	Fixed
The constant k in: $k \cdot [Stot]^n \cdot [FeOH3]^m$ (FeOH3 reduction)	-	450	113	45	4500	Fixed
The exponent n in: $k \cdot [Stot]^n \cdot [FeOH3]^m$ (FeOH3 reduction)	-	1.00	0.25	0.10	10.00	Fixed
The exponent m in: $k \cdot [Stot]^n \cdot [FeOH3]^m$ (FeOH3 reduction)	-	1.00	0.25	0.10	10.00	Fixed

Figure 132. Parameters to control iron precipitation chemistry

Iron can be reduced from its oxidized form (Ferric, Fe(III), Fe<sup>3+</sup>) to its reduced form (Ferrous, Fe(II), Fe<sup>2+</sup>), and oxidized back again.

#### 10.1.1.1 pH changes when adding iron salts

When ferrous and ferric is added to manage sulfide, the iron ion reacts with hydroxide ions in the water. In clean water, the reactions are:

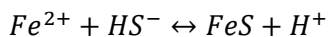


In other words, for each mole of ferrous, two moles of hydroxide are consumed, while three moles are consumed for each mole of ferric. Removing hydroxide from the water reduces the alkalinity, and this hence lowers the pH. The reduction of pH when adding iron salts can be quite substantial and become a problem for the efficiency of iron to manage sulfide in sewers.

In wastewater, the reduction of pH may be less than in clean water of the same buffer strength due to side reactions with carbonate and other charged substances in the water. Mega-WATS hence includes reduction factors for acid formation when dosing Fe(II) (ferrous) and Fe(III) (ferric) compared to theoretical values of 2 and 3, respectively (row 1 and 2, respectively, in the grid of Figure 131).

#### 10.1.1.2 Precipitation of ferrous sulfide

Fe(II) can precipitate with sulfide (S(II),  $\text{S}^{2-}$ ) and form iron sulfide (FeS) as:



In practice, it is not possible to reach the stoichiometric shown above, where 1 mole  $\text{Fe}^{2+}$  would result in 1 mole  $\text{S}^{2-}$  precipitated. The efficiency is lower because of side reactions occurring, where organic matter and carbonate might react with the iron. How much iron is lost to side reactions varies with the wastewater quality and with the pH. While the first is poorly understood, the second is understood in principle, as more iron is needed when pH becomes lower.

The exact relationship will depend on the wastewater characteristics, but an empirical molar ratio has been suggested as:

$$\text{if } \text{pH} < \text{p}K_{\text{FeRatio}} \text{ then } R_{\text{Fe:S}} = \Psi_{\text{FeS}} + a_{\text{FeRatio}}(\text{p}K_{\text{FeRatio}} - \text{pH})^{n_{\text{FeRatio}}} \text{ else } R_{\text{Fe:S}} = \Psi_{\text{FeS}}$$

The constant  $\text{p}K_{\text{FeRatio}}$  (row 5) is the limit above which the molar ratio equals  $\Psi_{\text{FeS}}$  (row 3)

$a_{\text{FeRatio}}$  and  $n_{\text{FeRatio}}$  are given in rows 4 and 6 of Figure 131.

The equation is in graphical form illustrated in Figure 132. Note that the numbers used to create the graph are an example only and might well differ from wastewater to wastewater.

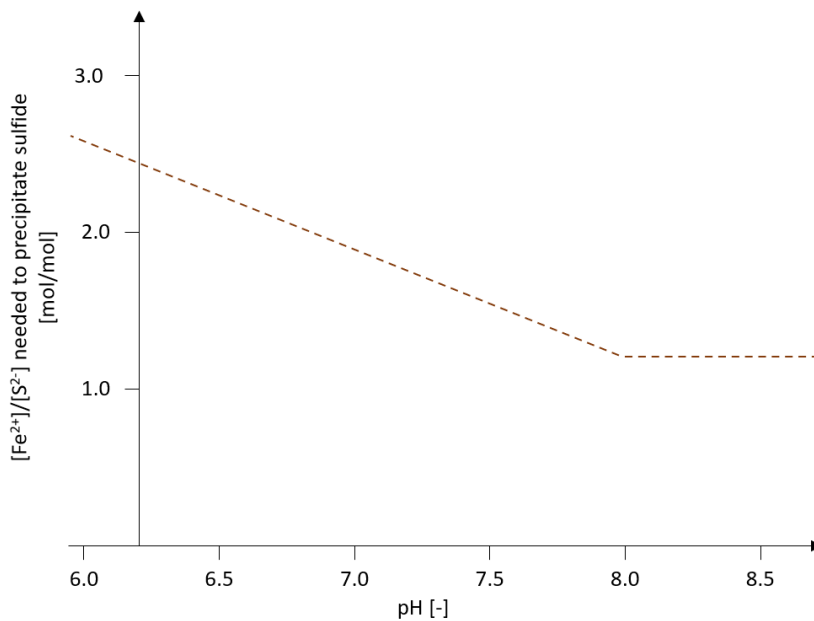


Figure 133. The principle of relationship between pH and efficiency, i.e., (mole Fe per mole S needed to precipitate sulfide, corresponding to the equation above).

The efficiency of the conversion of sulfide to ferrous sulfide (defined in the equation below) will depend on pH and wastewater type. The lower the pH, the lower the efficiency, i.e., the more sulfide will be left in the water without precipitating. This does though also depend on the molar ratio of iron to sulfide in the water.

$$C_{S(-II)} = \frac{[FeS]}{[FeS] + [S(-II)]}$$

The limit for conversion (i.e., the amount of S<sup>2-</sup> that is not precipitated even though there is Fe<sup>2+</sup> present) is empirically defined as:

$$S_{lim}^{2-} \geq ([S^{2-}] + [FeS]) \left(1 - \frac{R_M}{K_{RM} + R_M}\right) (1 - R_{M\_offset})$$

where

$$R_M = \frac{[Fe^{2+}] + [FeS]}{[S^{2-}] + [FeS]}$$

The value of the saturation constant  $K_{RM}$  is defined as being linearly dependent on pH defined by its value at pH 8.5 and 6.5 as the values 'Krm at pH 6.5' (row 7) and 'Krm at pH 8.5' (row 8), respectively, plus an offset from zero (row 9).

$$K_{RM} = a \text{ pH} + b$$

Note: When adding iron, pH decreases (section 10.1.1.1). The decrease in pH leads to poorer efficiency for the precipitation. This phenomenon puts an upper limit on how much iron should be added, as adding more iron would make the precipitation less efficient.

The process kinetics of the sulfide precipitation is simulated as:



$$\frac{d[S(-II)]}{dt} = -k_{FeSprecip} [S(-II)]^{n_{FeSprecip}} [FeOH_2]^{m_{FeSprecip}}$$

where sulfide and ferrous hydroxide is in the unit of mol/L

$k_{FeSprecip}$ ,  $n_{FeSprecip}$ , and  $m_{FeSprecip}$  are given in rows 10, 11, and 12 of Figure 131.

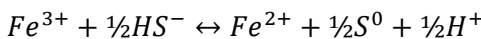
Iron sulfide (FeS) can be oxidized to form Fe(III), probably,  $S^0$  (elemental sulfur) plus maybe other oxidized sulfur compounds such as thiosulfate and sulfate. Oxidation of ferrous to ferric iron occurs when the wastewater becomes aerobic or chemical oxidants are added as discussed below.

#### 10.1.1.3 Precipitation of ferric sulfide

Direct precipitation of ferric sulfide can also occur and is seen in sewers. However, the process is not well understood and a simplified approach instead used where ferric first is reduced to ferrous (section 10.1.1.4) and then precipitates with sulfide (section 10.1.1.2).

#### 10.1.1.4 Reduction of ferric

The overall process of ferric to ferrous reduction is:



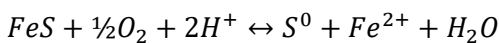
The process kinetics are simulated as fast as it is known that ferric is very efficient at removing sulfide:

$$\frac{dS_{FeOH_3}}{dt} = -k_{FeIIIreduc} S_{S(-II)}^{n_{FeIIIreduc}} X_{FeOH_3}^{m_{FeIIIreduc}}$$

$k_{FeIIIreduc}$ ,  $n_{FeIIIreduc}$ , and  $m_{FeIIIreduc}$  are given in rows 13, 14, and 15 of Figure 131.

#### 10.1.1.5 Oxidation of ferrous sulfide by oxygen

The overall process of FeS oxidation with elemental sulfur and Ferrous as the endpoint is:



It occurs in the water phase and biofilm. The process kinetics for the water phase is simulated as:

$$\frac{dFe_{FeS}}{dt} = k_{FeSoxO_2} \frac{S_O}{K_{FeSoxO_2} + S_O} \frac{X_{FeS}}{K_{FeO_2Fe} + X_{FeS}} X_H \alpha_w^{T-20} k_{H,pH}$$

The process kinetics for the biofilm is simulated as

$$\frac{dFe_{FeS}}{dt} = k_{FeSoxO_2} \frac{S_O}{K_{FeSoxO_2} + S_O} \frac{X_{FeS}}{K_{FeO_2Fe} + X_{FeS}} \epsilon_{Hf} X_{Hf} \frac{A_f}{V_w} \alpha_f^{T-20} k_{H,pH}$$

The parameters  $k_{FeSoxO_2}$ ,  $K_{FeSoxO_2}$ , and  $K_{FeO_2Fe}$  are given in the rows 1, 2, and 3 of the first grid in Figure 133.

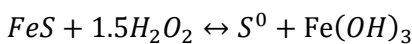
Oxidation of ferrous sulfide by oxygen only takes place above certain concentrations of oxygen and ferric sulfide, given in rows 4 and 5 of the first grid in Figure 133.

#### 10.1.1.6 Oxidation of ferrous sulfide by nitrate

Ferrous sulfide can be oxidized microbially with nitrate as electron acceptor, a process which for example has been shown for marine sediments. However, in sewer systems this process is believed to be slow and hence not included.

#### 10.1.1.7 Oxidation of ferrous sulfide by hydrogen peroxide

The overall process of sulfide oxidation by hydrogen peroxide is



assuming elemental sulfur as the endpoint of the oxidation.

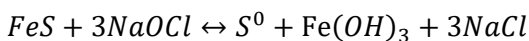
The process kinetics are described as

$$\frac{d[S(-II)]}{dt} = k_{S(-II)woxH_2O_2} [S(-II)]^{m_{S(-II)OXH_2O_2}} [H_2O_2]^{n_{S(-II)OXH_2O_2}} \alpha_{SoxChem}^{T-20}$$

The parameters  $k_{S(-II)woxH_2O_2}$ ,  $m_{S(-II)OXH_2O_2}$ , and  $n_{S(-II)OXH_2O_2}$  are in rows 1, 2, and 3 of the second grid in Figure 133. The yield constant of the oxidation is pH-dependent, with the yield being constant >pH 9 and <pH7, changing linearly between these. The yields at the two pH values are in rows 4 and 5 of the second grid in Figure 133.

#### 10.1.1.8 Oxidation of ferrous sulfide by hypochlorite

The overall process of sulfide oxidation by hypochlorite is:



assuming elemental sulfur and ferric iron as the endpoint of the oxidation.

The process kinetics are described as

$$\frac{d[S(-II)]}{dt} = k_{S(-II)woxOCl} [S(-II)]^{m_{S(-II)OXOCl}} [OCl]^{n_{S(-II)OXOCl}} \alpha_{SoxChem}^{T-20}$$

The parameters  $k_{S(-II)woxOCl}$ ,  $m_{S(-II)OXOCl}$ , and  $n_{S(-II)OXOCl}$  are in rows 1, 2, and 3 of the third grid in Figure 133. The yield constant of the oxidation is pH-dependent, with the yield being constant >pH 9 and <pH7, changing linearly between these. The yields at the two pH values are in rows 4 and 5 of the third grid in Figure 133.

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Process rate constant for FeS oxidation with O <sub>2</sub>	d <sup>-1</sup>	0.50	0.10	0.10	1.50	Fixed
Saturation constant for FeS oxidation with O <sub>2</sub> with respect to O <sub>2</sub>	gO <sub>2</sub> /m <sup>3</sup>	0.50	0.10	0.10	1.00	Fixed
Saturation constant for FeS oxidation with O <sub>2</sub> with respect to Fe	gS/m <sup>3</sup>	0.50	0.10	0.00	1.00	Fixed
Minimum oxygen concentration to allow FeS oxidation to proceed by O <sub>2</sub>	gO <sub>2</sub> /m <sup>3</sup>	0.50	0.10	0.00	1.00	Fixed
Minimum FeS concentration to allow FeS oxidation to proceed by O <sub>2</sub>	gS/m <sup>3</sup>	0.50	0.10	0.00	1.00	Fixed
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Process rate constant for FeS oxidation with H <sub>2</sub> O <sub>2</sub>	1/d	150	30	15	1500	Fixed
Process order of FeS concentration in FeS oxidation with H <sub>2</sub> O <sub>2</sub>	-	0.500	0.000	0.000	1.000	Fixed
Process order of H <sub>2</sub> O <sub>2</sub> concentration in FeS oxidation with H <sub>2</sub> O <sub>2</sub>	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for FeS oxidation with H <sub>2</sub> O <sub>2</sub> at pH 7	[Fe]/[H <sub>2</sub> O <sub>2</sub> ]	0.500	0.100	0.000	1.000	Fixed
Yield constant for FeS oxidation with H <sub>2</sub> O <sub>2</sub> at pH 9	[Fe]/[H <sub>2</sub> O <sub>2</sub> ]	0.125	0.100	0.000	1.000	Fixed
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Process rate constant for FeS oxidation with OCl	1/d	750	188	75	7500	Fixed
Process order of FeS concentration in FeS oxidation with OCl	-	0.500	0.000	0.000	1.000	Fixed
Process order of OCl concentration in FeS oxidation with OCl	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for FeS oxidation with OCl at pH 7	[Fe]/[OCl]	0.500	0.100	0.000	1.000	Fixed
Yield constant for FeS oxidation with OCl at pH 9	[Fe]/[OCl]	0.125	0.100	0.000	1.000	Fixed

Figure 134. Parameters to control iron oxidation chemistry

### 10.1.2 Nitrate and nitrite

Nitrate (NO<sub>3</sub><sup>-</sup>) as well as nitrite (NO<sub>2</sub><sup>-</sup>) induce anoxic heterotrophic oxidation of COD in the bulk water and biofilms of sewers. The compounds cause an increase in redox levels which inhibits the formation of hydrogen sulfide. Mega-WATS divides these processes into:

- Anoxic growth on NO<sub>3</sub><sup>-</sup> in bulk water
- Anoxic growth on NO<sub>2</sub><sup>-</sup> in bulk water
- Anoxic maintenance in bulk water when NO<sub>3</sub><sup>-</sup> is present
- Anoxic maintenance in bulk water when NO<sub>3</sub><sup>-</sup> is absent
- Anoxic growth in biofilm of NO<sub>3</sub><sup>-</sup>
- Anoxic growth in biofilm of NO<sub>2</sub><sup>-</sup>
- Anoxic hydrolysis in the bulk water
- Anoxic hydrolysis in the biofilm

The details of the processes are given in the file *WATS matrix*, which is an addendum to this manual. The parameters for these processes are entered in the grids shown in Figure 134 and Figure 135.

Simulation parameters						
Global parameters   Default COD   Default wastewater   Water aerobic het.   Biofilm aerobic het.   Sulfide form. biofilm   Sulfide form. water   Sulfide ox. aerobic   Sulfide ox. anoxic   Sulfide ox. gas Anaerobic ferm.   Bulk water anoxic   Biofilm anoxic   H2O2 Dosing   HOCl Dosing   Iron dosing   FeS ox.   Acid-base   Drops   Turbulences   Structures   Tracer						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Maximum growth rate of het. biomass utilizing NO <sub>3</sub> at 20°C (my)	1/d	1.00	0.50	0.20	6.00	Fixed
Maximum growth rate of het. biomass utilizing NO <sub>2</sub> in the presence of NO <sub>3</sub> at 20°C (my)	1/d	1.50	0.50	0.20	6.00	Fixed
Maximum growth rate of het. biomass utilizing NO <sub>3</sub> in the absence of NO <sub>3</sub> at 20°C (my)	1/d	1.50	0.50	0.20	6.00	Fixed
Yield constant for bulk water anoxic heterotrophic biomass (YHwNO)	mol e-eq/mol e-eq	0.450	0.050	0.100	0.600	Fixed
Saturation constant for het. growth on nitrate (KNO <sub>3</sub> )	gN/m <sup>3</sup>	0.600	0.200	0.200	10.000	Fixed
Saturation constant for het. growth on nitrite (KNO <sub>2</sub> )	gN/m <sup>3</sup>	0.300	0.100	0.100	10.000	Fixed
Maintenance rate during NO <sub>3</sub> respiration	1/d	0.083	0.050	0.010	0.800	Fixed
Maintenance rate during NO <sub>2</sub> respiration in the presence of NO <sub>3</sub>	1/d	0.125	0.050	0.010	0.800	Fixed
Maintenance rate during NO <sub>2</sub> respiration in the absence of NO <sub>3</sub>	1/d	0.125	0.050	0.010	0.800	Fixed
Relative hydrolysis under anoxic conditions compared to oxic condition (fryNOh)	-	0.60	0.10	0.40	1.00	Fixed
Saturation constant under anoxic conditions (KNO)	gNO/m <sup>3</sup>	0.500	0.100	0.100	2.000	Fixed

Figure 135. Parameters related to bulk water anoxic processes

Simulation parameters						
Global parameters   Default COD   Default wastewater   Water aerobic het.   Biofilm aerobic het.   Sulfide form. biofilm   Sulfide form. water   Sulfide ox. aerobic   Sulfide ox. anoxic   Sulfide ox. gas Anaerobic ferm.   Bulk water anoxic   Biofilm anoxic   H2O2 Dosing   HOCl Dosing   Iron dosing   FeS ox.   Acid-base   Drops   Turbulences   Structures   Tracer						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
½ order rate constant for biofilm, NO <sub>3</sub> reduction (k½NO <sub>3</sub> )	(gN/m) <sup>½</sup> 1/d	1.000	0.500	0.200	10.000	Fixed
½ order rate constant for biofilm, NO <sub>2</sub> reduction in the presence of NO <sub>3</sub> (k½NO <sub>2</sub> I)	(gN/m) <sup>½</sup> 1/d	1.500	0.500	0.300	10.000	Fixed
½ order rate constant for biofilm, NO <sub>2</sub> reduction in the absence of NO <sub>3</sub> (k½NO <sub>2</sub> II)	(gN/m) <sup>½</sup> 1/d	1.500	0.500	0.300	10.000	Fixed
Yield constant for biofilm biomass, anoxic conditions (YHfNO)	mol e-eq/mol e-eq	0.370	0.050	0.200	0.600	Fixed

Figure 136. Parameters related to biofilm anoxic processes

In addition to increasing the redox level, nitrate can biologically and chemically oxidize sulfide, albeit the process is somewhat slow. Mega-WATS divides these processes into:

- Sulfide oxidation, anoxic, chemical, bulk water
- Sulfide oxidation, anoxic, biological, bulk water
- Sulfide oxidation, anoxic, biological, biofilm

The details of the processes are given in the file 'WATS matrix' which is an addendum to this manual. These parameters are accessible via the grid shown in Figure 136.

Simulation parameters						
Anaerobic ferm. Bulk water anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Acid-base Drops Turbulences Structures Tracer Global parameters Default COD Default wastewater Water aerobic het. Biofilm aerobic het. Sulfide form. biofilm Sulfide form. water Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Rate constant for chemical oxidation of H2S (oxidation with NO2+NO3)	gH2S-S/(m3 d)	0.000200	0.000100	0.000000	0.010000	Fixed
Rate constant for chemical oxidation of HS- (oxidation with NO2+NO3)	gHS-S/(m3 d)	0.050000	0.010000	0.001000	1.000000	Fixed
Rate constant for biological oxidation of sulfide (oxidation with NO2+NO3)	gH2S-S/(m3 d)	0.500	0.100	0.010	10.000	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - bulk water (ox with NO2+NO3)	gS/gNO	2.574	0.286	1.430	5.720	Fixed
Stoichiometric reaction coefficient of biological sulfide oxidation - bulk water (ox with NO2+NO3)	gS/gNO	5.720	0.286	1.430	5.720	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - biofilm (ox with NO2+NO3)	gS/gNO	5.720	0.286	1.430	5.720	Fixed
Sulfide biofilm biological oxidation rate (ox with NO2+NO3)	gS/(m2 d)	0.500	0.050	0.005	5.000	Fixed
Sulfide bulk water chemical oxidation order with respect to sulfide (ox with NO2+NO3)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water chemical oxidation order with respect to NO2+NO3 (ox with NO2+NO3)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to sulfide (ox with NO2+NO3)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to NO2+NO3 (ox with NO2+NO3)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to sulfide (ox with NO2+NO3)	-	0.500	0.100	0.000	1.000	Fixed

Figure 137. Parameters related to anoxic sulfide oxidation

The rate of the chemical sulfide oxidation by nitrate and nitrite depends on pH as there is one rate for the oxidation of H<sub>2</sub>S and another for oxidation of HS<sup>-</sup>. The oxidation is then a power function of dissolved sulfide (S(-II)) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and nitrate plus nitrite (S<sub>NO</sub>):

$$\frac{d[S(-II)]}{dt} = \frac{k_{H_2S} S_{wcNO} + k_{HS^-} S_{wcNO} \frac{K_{a1}}{0.1^{pH}}}{1 + \frac{K_{a1}}{0.1^{pH}}} S_{S(-II)}^{mwcNO} S_{NO}^{nwcNO} \alpha_{SoxcNO}^{T-20}$$

The rate of biological sulfide oxidation by nitrate and nitrite in the bulk water is described as a power function of dissolved sulfide (S(-II)) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and nitrate plus nitrite (S<sub>NO</sub>):

$$\frac{d[S(-II)]}{dt} = k_{S(-II)w} S_{S(-II)}^{mwbNO} (S_{NO3} + S_{NO2})^{nwbNO} \alpha_{SoxbNO}^{T-20} k_{S(-II),pH}$$

The rate of biological sulfide oxidation by nitrate and nitrite in the biofilm is described as a power function of dissolved sulfide (S(-II)) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and nitrate plus nitrite (S<sub>NO</sub>):

$$\frac{d[S(-II)]}{dt} = k_{S(-II)f} S_{S(-II)}^{mfbNO} (S_{NO3} + S_{NO2})^{nfbNO} \frac{A_f}{V_w} \alpha_{SoxbNO}^{T-20} k_{S(-II),pH}$$

### 10.1.3 Oxygen

Oxygen can be injected into the wastewater as pure oxygen or as air. In most cases such injection takes place in force mains. The aeration of wastewater in a gravity main can be seen as passive oxygen addition.

Whatever the cause for the oxygen in the wastewater, it will react with the sulfide herein. When used to

manage sulfide, oxygen causes an increase in redox levels which inhibit the formation of hydrogen sulfide. Mega-WATS divides the processes into:

- Aerobic growth in the bulk water
- Aerobic maintenance in the bulk water
- Aerobic growth in the biofilm
- Aerobic hydrolysis in the bulk water
- Aerobic hydrolysis in the biofilm

The details of the processes are given in the file 'WATS matrix' which is an addendum to this manual. The parameters for these processes are entered in the grids shown in Figure 137 and Figure 138.

Simulation parameters						
Anaerobic ferm.   Bulk water anoxic   Biofilm anoxic   H2O2 Dosing   HOCl-Dosing   Iron dosing   FeS ox.   Acid-base   Drops   Turbulences   Structures   Tracer Global parameters   Default COD   Default wastewater   Bulk water aerobic   Biofilm aerobic   Sulfide form. biofilm   Sulfide form. water   Sulfide ox. aerobic   Sulfide ox. anoxic   Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Maximum growth rate of the heterotrophic biomass at 20°C (my)	1/d	6.00	2.00	2.00	15.00	Fixed
Yield constant for bulk water aerobic heterotrophic biomass (YHwO2)	mol e-eq/mol e-eq	0.550	0.050	0.300	0.800	Fixed
Saturation constant for readily biodegradable substrate (KS)	gCOD/m3	1.00	0.20	0.10	10.00	Fixed
Saturation constant for dissolved oxygen (KO)	gO2/m3	0.100	0.050	0.010	1.000	Fixed
Maintenance energy rate constance at 20°C (qm)	1/d	0.500	0.200	0.100	2.000	Fixed
Minimum maintenance energy rate constance at 20°C (qmMin)	1/d	0.125	0.050	0.025	0.500	Fixed
Rate constant for fast hydrolysable substrate at 20°C (kh,fast)	1/d	4.000	1.200	1.000	15.000	Fixed
Saturation constant (KX,fast) for kh,fast depends on kh,fast with the slope (no dependency = zero)	gCOD/gCOD	0.230	0.050	0.050	1.000	Fixed
and with the intersection (if no dependency, then this is equal to KX,fast)	gCOD/gCOD	-0.500	0.100	-1.000	-0.001	Fixed
Rate constant for medium hydrolysable substrate at 20°C (kh,med)	1/d	1.000	0.500	0.500	3.000	Fixed
Saturation constant (KX,med) for kh,med depends on kh,med with the slope (no dependency = zero)	gCOD/gCOD	0.230	0.050	0.000	1.000	Fixed
Saturation constant (KX,med) for kh,med depends on kh,med with the slope (no dependency = zero)	gCOD/gCOD	-0.500	0.100	-1.000	-0.001	Fixed
Rate constant for slow hydrolysable substrate at 20°C (kh,slow)	1/d	0.50	0.30	0.10	3.00	Fixed
Saturation constant for slow hydrolysable substrate (KX,slow)	gCOD/gCOD	0.900	1.300	0.010	5.000	Fixed
Arrhenius constant for the bulk water heterotrophic transformations (alpha_w)	-	1.070	0.010	1.000	1.150	Fixed
Parameter accouting for the width of the biological heterotrophic pH dependency	-	175.00	20.00	20.00	1000.00	Fixed

Figure 138. Parameters related to bulk water aerobic processes

Simulation parameters						
Anaerobic ferm. Bulk water anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Acid-base Drops Turbulences Structures Tracer Global parameters Default COD Default wastewater Bulk water aerobic <b>Biofilm aerobic</b> Sulfide form. biofilm Sulfide form. water Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
½ order rate constant for biofilm, aerobic conditions ( $k_{1/2O_2}$ )	(gO <sub>2</sub> /m) <sup>1/2</sup> 1/d	6.000	2.000	2.000	100.000	Fixed
Yield constant for biofilm biomass, aerobic conditions (Y <sub>HfO<sub>2</sub></sub> )	gCOD/gCOD	0.550	0.050	0.400	0.800	Fixed
Saturation constant for biofilm organic substrate	gCOD/m <sup>3</sup>	4.00	2.00	0.10	20.00	Fixed
Biofilm biomass efficiency constant (epsilon)	-	0.30	0.10	0.10	0.60	Fixed
Biofilm biomass concentration (X <sub>B, film</sub> )	gCOD/m <sup>2</sup>	10.0	1.0	1.0	100.0	Fixed
Arrhenius constant for the biofilm heterotrophic transformations (alpha <sub>f</sub> )	-	1.050	0.010	1.000	1.100	Fixed

Figure 139. Parameters related to biofilm aerobic processes

In addition to increasing the redox level, oxygen can biologically and chemically oxidize sulfide. Mega-WATS divides these processes into:

- Sulfide oxidation, aerobic, chemical, bulk water
- Sulfide oxidation, aerobic, biological, bulk water
- Sulfide oxidation, aerobic, biological, biofilm

The details of the processes are given in the file 'WATS matrix' which is an addendum to this manual. The parameters for these processes are entered in the grid shown in Figure 139.



Simulation parameters						
Anaerobic ferm. Bulk water anoxic Biofilm anoxic H2O2 Dosing HOCl Dosing Iron dosing FeS ox. Acid-base Drops Turbulences Structures Tracer Global parameters Default COD Default wastewater Bulk water aerobic Biofilm aerobic Sulfide form. biofilm Sulfide form. water Sulfide ox. aerobic Sulfide ox. anoxic Sulfide ox. gas						
Parameter	Unit	Mean	StDev	Min	Max	Distribution
Rate constant for chemical oxidation of H2S (oxidation with O2)	gH2S-S/(m3 d)	0.960	0.240	0.010	100.000	Fixed
Rate constant for chemical oxidation of HS <sup>-</sup> (oxidation with O2)	gHS-S/(m3 d)	12.000	2.400	0.100	100.000	Fixed
Rate constant for biological oxidation of sulfide	gH2S-S/(m3 d)	12.000	2.400	0.100	100.000	Fixed
pH optimum for heterotrophic and autotrophic processes	-	7.5	1.0	6.5	8.5	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - bulk water (ox with O2)	gS/gO2	0.900	0.100	0.500	2.000	Fixed
Stoichiometric reaction coefficient of biological sulfide oxidation - bulk water (ox with O2)	gS/gO2	2.000	0.100	0.500	2.000	Fixed
Stoichiometric reaction coefficient of chemical sulfide oxidation - biofilm (ox with O2)	gS/gO2	2.000	0.100	0.500	2.000	Fixed
Sulfide biofilm biological oxidation rate (ox with O2)	gS/(m2 d)	2.400	0.240	0.240	48.000	Fixed
Sulfide bulk water chemical oxidation order with respect to sulfide (ox with O2)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water chemical oxidation order with respect to oxygen (ox with O2)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to sulfide (ox with O2)	-	1.000	0.100	0.000	1.000	Fixed
Sulfide bulk water biological oxidation order with respect to oxygen (ox with O2)	-	0.100	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to sulfide (ox with O2)	-	0.500	0.100	0.000	1.000	Fixed
Sulfide biofilm oxidation order with respect to oxygen (ox with O2)	-	0.500	0.100	0.000	1.000	Fixed
Parameter accounting for the width of the biological sulfide oxidation pH dependency	-	25.00	5.00	10.00	100.00	Fixed
Arrhenius constant for the chemical oxidation of sulfide	-	1.070	0.010	1.000	1.150	Fixed
Arrhenius constant for the biological oxidation of sulfide in the bulk water	-	1.070	0.010	1.000	1.100	Fixed

Figure 140. Parameters related to aerobic sulfide oxidation

The rate of the chemical sulfide oxidation by oxygen depends on pH as there is one rate for the oxidation of H<sub>2</sub>S and another for oxidation of HS<sup>-</sup>. The oxidation is then a power function of dissolved sulfide (S(-II) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and oxygen (S<sub>0</sub>):

$$\frac{d[S(-II)]}{dt} = \frac{k_{H_2S_{wcO_2}} + k_{HS^-_{wcO_2}} \frac{K_{a1}}{0.1^{pH}}}{1 + \frac{K_{a1}}{0.1^{pH}}} S_{S(-II)}^{m_{wcO_2}} S_O^{n_{wcO_2}} \alpha_{Sox_{cO_2}}^{T-20}$$

The rate of biological sulfide oxidation by oxygen in the bulk water is described as a power function of dissolved sulfide (S(-II) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and oxygen (S<sub>0</sub>):

$$\frac{d[S(-II)]}{dt} = k_{S(-II)_{wOx_{bO_2}}} S_{S(-II)}^{m_{wbO_2}} S_O^{n_{wbO_2}} \alpha_{Sox_{bO_2}}^{T-20} k_{S(-II),pH}$$

The rate of biological sulfide oxidation by oxygen in the biofilm is described as a power function of dissolved sulfide (S(-II) (H<sub>2</sub>S + HS<sup>-</sup> + S<sup>2-</sup>) and oxygen (S<sub>0</sub>):

$$\frac{d[S(-II)]}{dt} = k_{S(-II)_{fOx_{bO_2}}} S_{S(-II)}^{m_{fbO_2}} S_O^{n_{fbO_2}} \frac{A_f}{V_w} \alpha_{Sox_{bO_2}}^{T-20} k_{S(-II),pH}$$

#### 10.1.4 Hydrogen peroxide

Hydrogen peroxide is a strong oxidizer which affects many reduced substances in the wastewater. It oxidizes sulfide, which is typically why it is added, it oxidizes ferrous sulfide (section 10.1.1.7), and it oxidizes COD including other malodorous substances than hydrogen sulfide.

$$\frac{d[S(-II)]}{dt} = k_{S(-II)woxH_2O_2} S_{S(-II)}^{m_{S(-II)OxH_2O_2}} S_{H_2O_2}^{n_{S(-II)OxH_2O_2}} \alpha_{SoxChem}^{T-20}$$

The details of the processes are given in the file 'WATS matrix' which is an addendum to this manual. The parameters for these processes are entered in the grid shown in Figure 140.

##### 10.1.4.1 Oxidation of sulfide by hydrogen peroxide

The overall process of sulfide oxidation by hydrogen peroxide is  $H_2S + H_2O_2 \leftrightarrow S^0 + 2H_2O$  assuming elemental sulfur as the endpoint of the oxidation.

$$\frac{d[S(-II)]}{dt} = \frac{d[S(-II)]}{dt} = k_{S(-II)woxH_2O_2} [S(-II)]^{m_{S(-II)OxH_2O_2}} [H_2O_2]^{n_{S(-II)OxH_2O_2}} \alpha_{SoxChem}^{T-20}$$

The yield constant of the oxidation is pH-dependent, with the yield being constant >pH 9 and <pH7, changing linearly between these.

##### 10.1.4.2 Oxidation of ferrous sulfide by hydrogen peroxide

See section 10.1.1.7.

##### 10.1.4.3 Oxidation of COD by hydrogen peroxide

The overall process of sulfide oxidation by hydrogen peroxide is  $COD + H_2O_2 \rightarrow xCO_2 + yH_2O + \dots$ . The actual endpoint of the oxidation is not known. It seems likely that endpoints depend on the organic substance, and that not all endpoints are fully mineralized substances. Nevertheless, and due to this lack of scientific knowledge, all COD fractions are assumed to be oxidized to the same extent and products are fully mineralized substances (CO<sub>2</sub>, H<sub>2</sub>O, etc.)

$$\frac{d[COD_{tot}]}{dt} = k_{CODwoxH_2O_2} [COD_{tot}]^{p_{CODOxH_2O_2}} [H_2O_2]^{q_{CODOxH_2O_2}} \alpha_{SoxChem}^{T-20}$$

The yield constant of the oxidation is pH-dependent, with the yield being constant >pH 9 and <pH7, changing linearly between these.

#### 10.1.4.4 Oxidation of methyl mercaptan by hydrogen peroxide

The overall process rate of methyl mercaptan oxidation by hydrogen peroxide is  $CH_4S + 4H_2O_2 \rightarrow S^0 + CO_2 + 6H_2O$ , assuming elemental sulfur as the end point of the sulfur oxidation. The rate equation is:

$$\frac{d[MM]}{dt} = k_{MMwoxH2O2} [COD_{tot}]^{p_{MMoxH2O2}} [H_2O_2]^{q_{MMoxH2O2}} \alpha_{SoxChem}^{T-20}$$

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Process rate constant in sulfide oxidation with [H2O2]	1/d	50	13	5	500	Fixed
Process order of sulfide concentration in sulfide oxidation with [H2O2]	-	0.500	0.000	0.000	1.000	Fixed
Process order of H2O2 concentration in sulfide oxidation with [H2O2]	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for sulfide oxidation with H2O2 at pH 7	[S]/[H2O2]	1.000	0.000	0.000	1.000	Fixed
Yield constant for sulfide oxidation with H2O2 at pH 9	[S]/[H2O2]	0.250	0.000	0.000	1.000	Fixed
Process rate constant for COD oxidation with H2O2	1/d	4.0	0.0	0.0	0.0	Fixed
Process order of COD concentration in COD oxidation with H2O2	-	0.500	0.000	0.000	1.000	Fixed
Process order of H2O2 concentration in COD oxidation with H2O2	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for COD oxidation with H2O2 at pH 7	[COD]/[H2O2]	0.500	0.100	0.000	1.000	Fixed
Yield constant for COD oxidation with H2O2 at pH 9	[COD]/[H2O2]	0.125	0.100	0.000	1.000	Fixed
Process rate constant for methyl mercaptan oxidation with H2O2	1/d	30.0	0.0	0.0	0.0	Fixed
Process order of methyl mercaptan concentration in methyl mercaptan oxidation with H2O2	-	0.500	0.000	0.000	1.000	Fixed
Process order of H2O2 concentration in methyl mercaptan oxidation with H2O2	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for methyl mercaptan oxidation with H2O2 at pH 7	[MM]/[H2O2]	1.000	0.100	0.000	1.000	Fixed
Yield constant for methyl mercaptan oxidation with H2O2 at pH 9	[MM]/[H2O2]	1.000	0.100	0.000	1.000	Fixed
Saturation constant inhibiting biofilm fermentation in the presense of H2O2	mgH2O2/L	0.500	0.100	0.050	5.000	
Saturation constant inhibiting bulk water fermentation in the presense of H2O2	mgH2O2/L	0.100	0.020	0.010	1.000	
Saturation constant inhibiting biofilm sulfide formation in the presense of H2O2	mgH2O2/L	0.500	0.100	0.050	5.000	
Saturation constant inhibiting bulk water sulfide formation in the presense of H2O2	mgH2O2/L	0.100	0.020	0.010	1.000	

Figure 141. Parameters related to oxidation by hydrogen peroxide. See also Figure 133, second grid

#### 10.1.5 Hypochlorite

Hypochlorite is a strong oxidant and, like other strong oxidants, readily oxidizes any reduced constituent present including sulfide, CO, and ferrous sulfide. Hypochlorite reactions are analogous to those of hydrogen peroxide. The parameters are shown in Figure 141.

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Process rate constant in sulfide oxidation with [OCI-]	1/d	600	150	60	6000	Fixed
Process order of sulfide concentration in sulfide oxidation with [OCI-]	-	0.500	0.000	0.000	1.000	Fixed
Process order of OCI concentration in sulfide oxidation with [OCI-]	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for sulfide oxidation with OCI- at pH 7	[S]/[OCI-]	0.500	0.000	0.000	1.000	Fixed
Yield constant for sulfide oxidation with OCI- at pH 9	[S]/[OCI-]	0.125	0.000	0.000	1.000	Fixed
Process rate constant for COD with OCI	1/d	20.000	5.000	2.000	200.000	Fixed
Process order of COD concentration in COD oxidation with OCI	-	0.500	0.000	0.000	1.000	Fixed
Process order of OCI concentration in COD oxidation with OCI	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for COD oxidation with OCI at pH 7	[COD]/[OCI-]	0.250	0.100	0.000	1.000	Fixed
Yield constant for COD oxidation with OCI at pH 9	[COD]/[OCI-]	0.063	0.100	0.000	1.000	Fixed
Process rate constant for MM with OCI	1/d	150.000	37.500	15.000	1500.000	Fixed
Process order of MM concentration in MM oxidation with OCI	-	0.500	0.000	0.000	1.000	Fixed
Process order of OCI concentration in MM oxidation with OCI	-	0.100	0.000	0.000	1.000	Fixed
Yield constant for MM oxidation with OCI at pH 7	[MM]/[OCI-]	1.000	0.100	0.000	1.000	Fixed
Yield constant for MM oxidation with OCI at pH 9	[MM]/[OCI-]	1.000	0.100	0.000	1.000	Fixed
Saturation constant inhibiting biofilm fermentation in the presense of OCI	mgOCI/L	0.500	0.100	0.050	5.000	Fixed
Saturation constant inhibiting bulk water fermentation in the presense of OCI	mgOCI/L	0.100	0.020	0.010	1.000	Fixed
Saturation constant inhibiting biofilm sulfide formation in the presense of OCI	mgOCI/L	0.500	0.100	0.050	5.000	Fixed
Saturation constant inhibiting bulk water sulfide formation in the presense of OCI	mgOCI/L	0.100	0.020	0.010	1.000	Fixed

Figure 142. Parameters related to oxidation by hypochlorite. See also Figure 133, second grid

### 10.1.6 Base

Base is added as moles of OH<sup>-</sup>

### 10.1.7 Magnesium hydroxide

Magnesium hydroxide is a salt of low solubility. Added to water, it stabilizes the pH as it slowly dissolves. The pH is governed by the buffer system in combination with the magnesium solubility product:

$$K_{SP} = [Mg^{2+}][OH^{-}]^2$$

In most literature,  $K_{SP}$  is set to  $5.61 \times 10^{-12}$

In Mega-WATS, the value  $pK_{SP}$  is given, defined as  $pK_{SP} = -\log(K_{SP})$  and corresponding to  $pK_{SP} = 11.251$

## 10.2 Adding chemicals during run-time

Dosing of chemicals can be done via the dosing file (section 4.2.5), which is the option of choice if a known dosing is to be implemented. However, when testing different dosing options, it is more convenient do this during run-time using the GUI.

Chose a pipe in before opening the run-time dosing menu. In the lower left corner of the main form, there is a button called *Dose to:* To the right of it is the name of the pipe (and its number). Press the button and a dosing menu opens (Figure 142).

- Chose the chemical to dose
- Chose the dose unit
- Press the *Dose* button

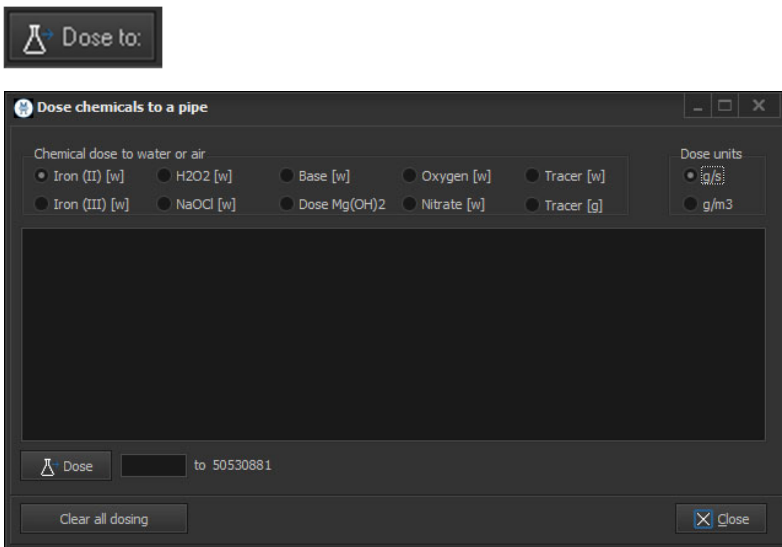


Figure 143. Menu for run-time dosing of chemicals

Pressing the *Clear all dosing* button will clear all dosing, also those loaded via a dosing file (section 4.2.5).

Run Mega-WATS and check out the result.

### 10.3 Auto-calibrating chemical dosing

Optimizing dosing of chemicals to several dosing stations at once can be semi-automated in Mega-WATS. Note that this is solely meant as a help for experts and not a silver bullet. Less experienced sewer process modelers should optimize dosing manually. Mega-WATS has an option for automatic dosing of chemicals where 15 dosing points can be optimized in one go. Chose '*Calibration*' -> '*Auto calibrate chemical dosing*' for the auto-calibration (Figure 143). This can be done before or after having run the model. It is though easier to first run Mega-WATS once.

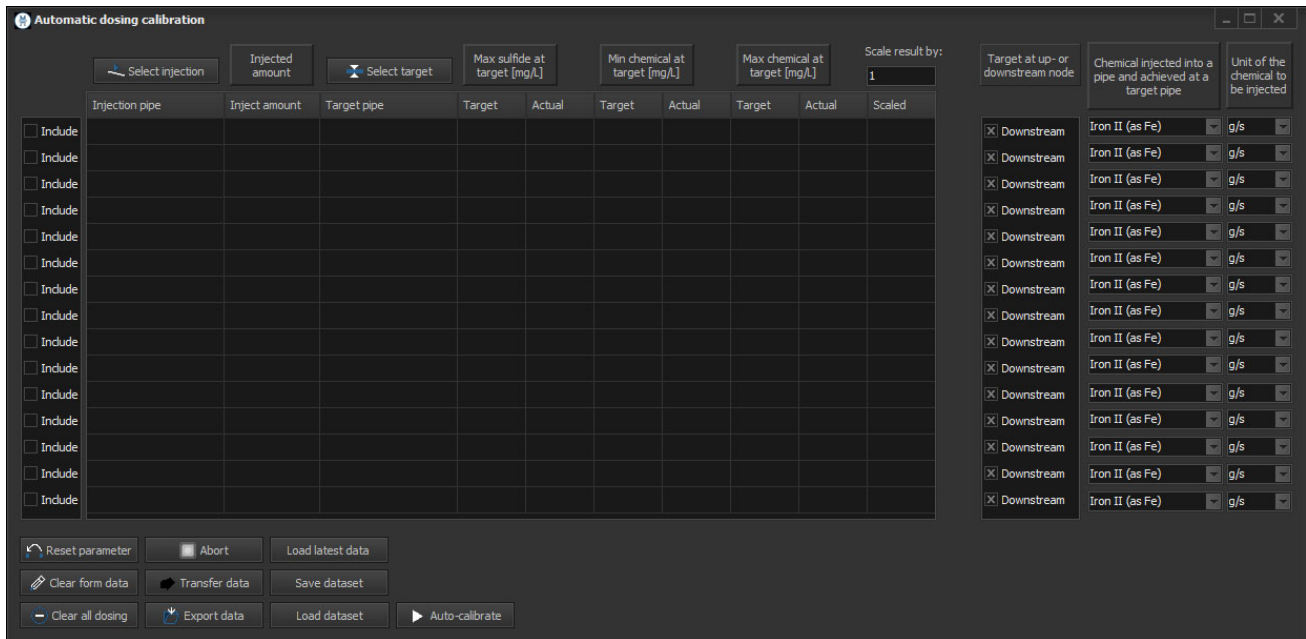


Figure 144. Auto-calibration menu for dosing of chemicals

The procedure is:

- Select the pipe on the map where you want the injection to occur (at its upstream end)
- Click the button 'Select injection'. This transfers the name of the selected pipe to the first column of the chosen row.
- Select an injection pipe automatically checks the box ' Include'. Unchecking it results in this pipe being ignored in the calibration.
  - You can also write the name manually or copy it from somewhere else using Ctrl-c and Ctrl-v. Remember to check ' Include', otherwise this pipe is not included in the calibration.
- Select the pipe on the map where you want the target to be evaluated.
- Click the button 'Select target'. This transfers the name of the selected pipe to the third column of the chosen row.
- Decide whether the target is the up- or downstream end of this pipe. If it is the downstream end, then check the box to the right of the grid ( Downstream). It is checked as default, meaning that the default target is the downstream end of the pipe.
- Select the chemical to inject from the drop-down list on the right.
- Select whether the unit of dosing is in flux (g/s (mol/s for base)) or concentration (g/m<sup>3</sup> (mol/m<sup>3</sup> for base))
- Select the initial amount to dose. When choosing an injection pipe, this cell is populated by '1', however, the closer to the actual value is the initial selection, the faster will be the calibration. Hence, and especially for large networks with a long simulation time, it is preferred to initialize with as realistic a value as possible.
- Select the maximum sulfide concentration at the target. Note then when selecting Magnesium Hydroxide or Base as chemicals, this will not necessarily hinder the formation of sulfide, as these chemicals act to increase the pH and hereby hinder H<sub>2</sub>S-release into the sewer air. For these chemicals, the max sulfide concentration at the target should hence be set to a high value.
- Select the minimum concentration of chemical at the target. One typically wants some leftover chemical at the target, but zero can also be selected.

- Select the maximum concentration of chemical at the target. One typically wants some leftover chemical at the target, but zero can also be selected.

In case a pipe experiences injection of two different chemicals, the mode of the dosing must be identical for the two (or more) injections. I.e., either g/m<sup>3</sup> and mole/m<sup>3</sup> or g/s and mole/s.

Press the *Auto-calibrate* bottom (Figure 144). The iteration now runs until the set targets are reached. Note that if the set targets cannot be reached, the iteration just goes on and on! In such case press the *Abort* button to stop the simulation.

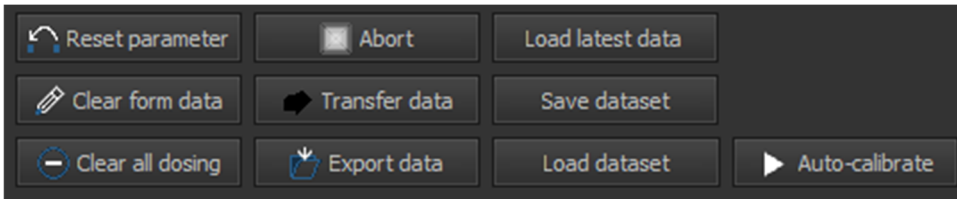


Figure 145. Buttons on the chemicals auto-calibration form

The function of the buttons in the lower left corner of the form (Figure 144):

- *Reset parameters* values of the grid to what they were before the auto-calibration.
- *Clear form data* deletes all content from the grid
- *Clear all dosing* clears all dosing, also those loaded via a dosing file (section 4.2.5).
- *Abort* interrupts the calibration
- *Transfer data* transfers the data from the calibration to the dosing window of the main form. Note that it is not the text in the grid per se which is moved, but the data contained in the memory. Hence, changing a cell manually and then pressing *Transfer data* will not have any affect.
- *Export data* creates an export to a Tab-separated text file
- *Load latest data* loads the result of the last calibration run into the grid
- *Save dataset* saves calibration data from the grid to an untyped file with the extension .adc
- *Load dataset* loads a saved dataset stored in an untyped file with the extension .adc into the grid
- *Auto-calibrate* starts a calibration run

## 11 Stochastic simulation

### 11.1 What stochastic simulation does

Mega-WATS can run stochastic simulations applying a Monte Carlo Method. Monte Carlo Simulation is a technique which is used to estimate the possible outcomes of an uncertain event. A Monte Carlo Simulation lies in the intersection of probabilistic and deterministic modelling as it applies probability distributed parameters to a deterministic model.

Mega-WATS is a deterministic model, i.e., a model where quantification is based on calculated parameters. A deterministic model is a mathematical description of a system in which relationships are fixed (i.e., taking no account of probability), so that any given input invariably yields the same result. A simple example is to assume that for a given population, the height of males is a factor times the height of females, which could be described as  $h_{male} = \alpha h_{female}$  with  $\alpha$  being a constant. This is however only true for the average heights of the population. Such approach is what Mega-WATS uses, assuming deterministic relationships between



many parameters. In other words, Mega-WATS predicts what can be expected on average applying a given set of model parameters.

In the example of the height of females and males, one can introduce a female height probability distribution instead of a fixed female height. Let's call that  $p(h_{female})$ . Applying the previous equation, this leads to a calculated probability distribution of the male height.

In the example, it is simple to find the male height probability distribution solving the equation analytically. However, when having a deterministic model which consists of many coupled equations, a numerical solution is needed. This is where the Monte Carlo Method comes in. First a deterministic model is set up, then random values are drawn from the probability distribution of each parameter, then the model is run. This process is repeated many times. The output of each run constitutes a point in the output probability distribution function.

Stochastic simulations can be used for several things, for example:

- Compare modeled and measured simulation outcomes
- Decide which model parameters are sensitive and which are less so to the simulation outcome.
- Assess how strongly a certain parameter affects a certain outcome
- Assess how the variation of a specific parameter will affect a specific outcome

The Achilles heel of this approach is that the probability distribution of each parameter must be known. Such distributions have been measured for very few parameters, and under sewer conditions only for a handful. They are hence estimated and often simply guesstimated. Nevertheless, a Monte Carlo Simulation has for example been shown to yield good results when comparing to distributions of H<sub>2</sub>S-gas in the sewer air, where thousands of individual datapoints typically are available.

## 11.2 How Mega-WATS implements stochastic simulation

In the case of Mega-WATS, there are hundreds of parameters involved in the model, and each can be assigned a distribution. The allowed distributions are fixed, normal, log-normal, and linear. If 'fixed' is chosen, the parameter is not varied between runs. If one of the other distributions are chosen, the parameter is drawn from this distribution by means of a random number generator. The output to be presented is chosen before the run, as the amount of possible output is very large.

The distributions are set in the simulation parameter form (Figure 145). As default, the left side of the grid contains the word 'Fixed'. If one of these cells is right or left click, a menu holding the possible distributions pops up. Then one checks the desired distribution.

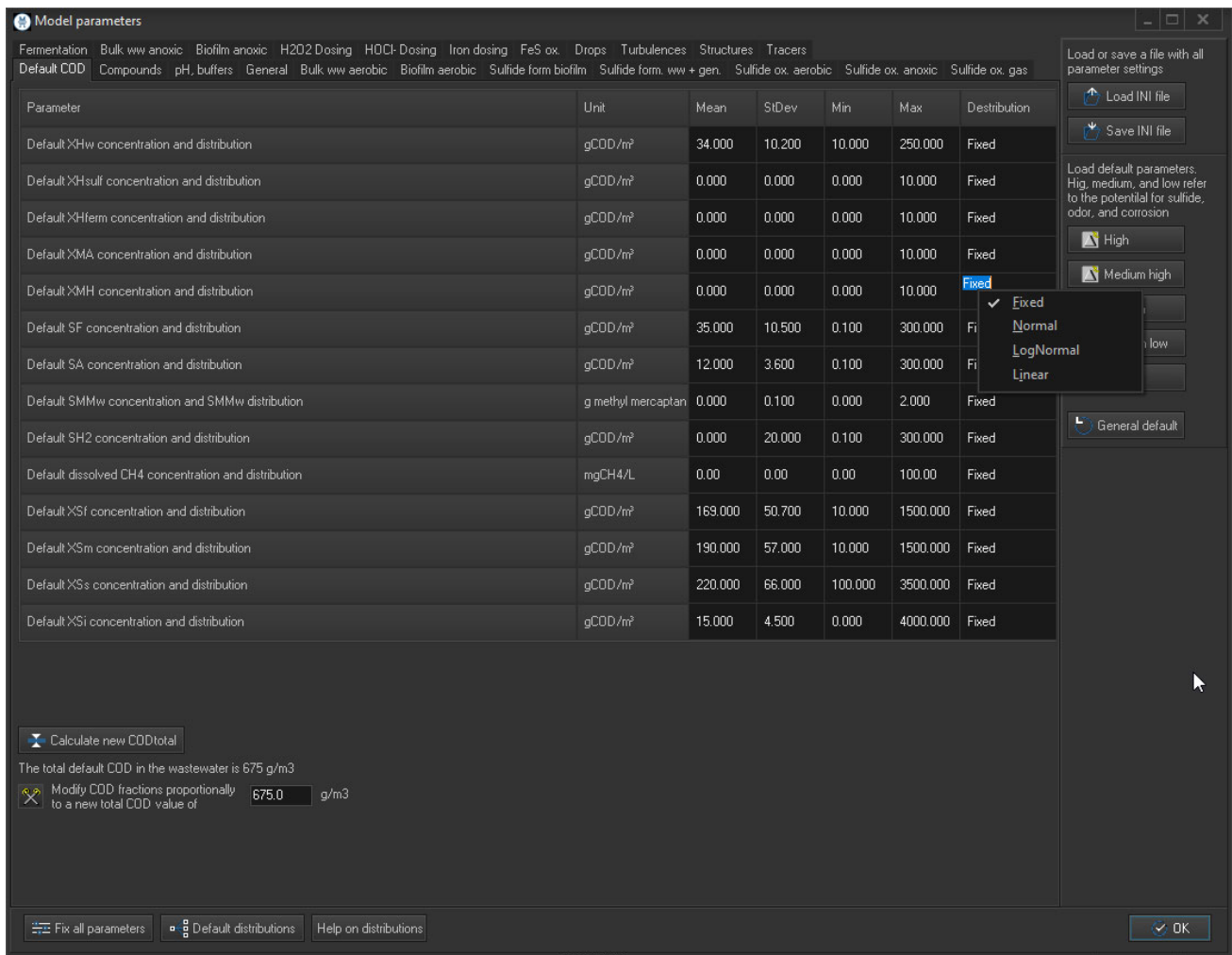


Figure 146. Setting distributions and their values – example of one of the input forms.

As Mega-WATS has many parameters, manually checking each before a run becomes tedious. Hence there are two buttons for quick choices, one changes all distributions to fixed and one that sets a predefined set of default ones for all parameters in the *Model parameters* form.

Besides the distribution type, each row holds the parameters Mean, StDev, Min, Max. The values Min and Max define the upper and lower boundary the value can have during a simulation. For the example temperature in Figure 145, where the allowed minimum temperature of the water is 0°C while the allowed maximum temperature is 100°C. The mean is in this example set to 22°C with a standard deviation of 2°C. When choosing normal as the probability distribution, this means that the temperature for each run is drawn from a normal distribution with 22°C as mean and 2°C as standard deviation.

### 11.3 An example of stochastic modelling

Running Mega-WATS 1,000 times on a small catchment (25 km of pipe, hereof 4.8 km force mains) with temperature set to normal distributed while all other parameters are kept fixed, results in the sulfide distribution at the discharge of the catchment shown in Figure 146. It is obvious that the output distribution is not normal like the temperature was, but slightly skewed.

Running Mega-WATS 1,000 times on the same small catchment but this time with parameters set to default distributions yields a more diverse picture (Figure 147). The 1,000 runs no longer yield a smooth distribution,

and more runs might well be needed. It is also clear that there are extreme outliers. While the mean and the median of the first set of simulations was nearly the same (1.886 versus 1.847), they differed somewhat in the second set of simulations (1.763 versus 1.475).

Increasing the number of model-runs to 10,000 yields a much smoother distribution (Figure 148) where a long tail towards high extreme concentrations is clearly visible. Looking at the mean and the median of doing 1,000 runs versus 10,000 runs shows that these values are little affected (1.784 versus 1.508). The difference for the parameters is only 2.2% in terms of the median value, 5.5% of the 25<sup>th</sup> percentile and 0.8% in terms of the 75<sup>th</sup> percentile. In most cases it hence is overkill to run so many simulations.

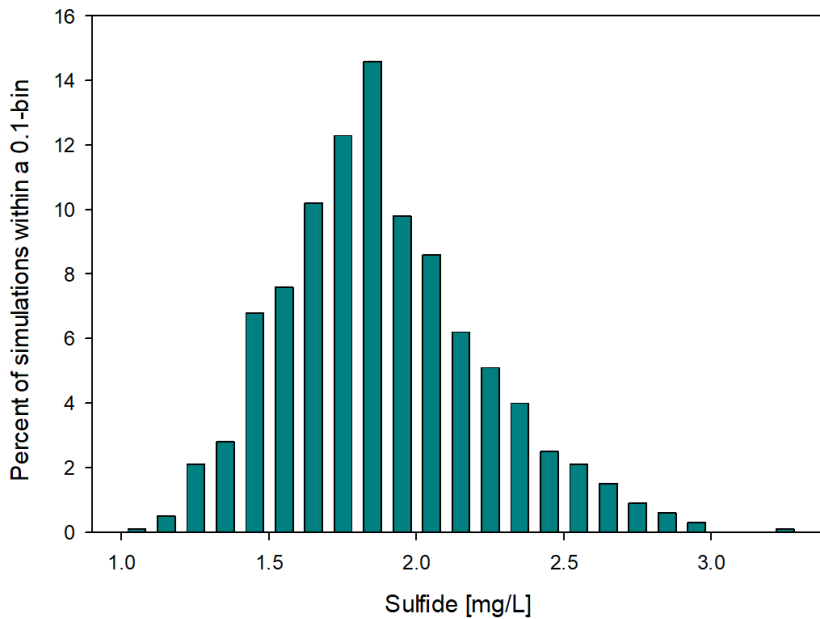


Figure 147. An example of the outcome of a Monte Carlo Simulation varying only one parameter, namely the temperature; 1,000 runs

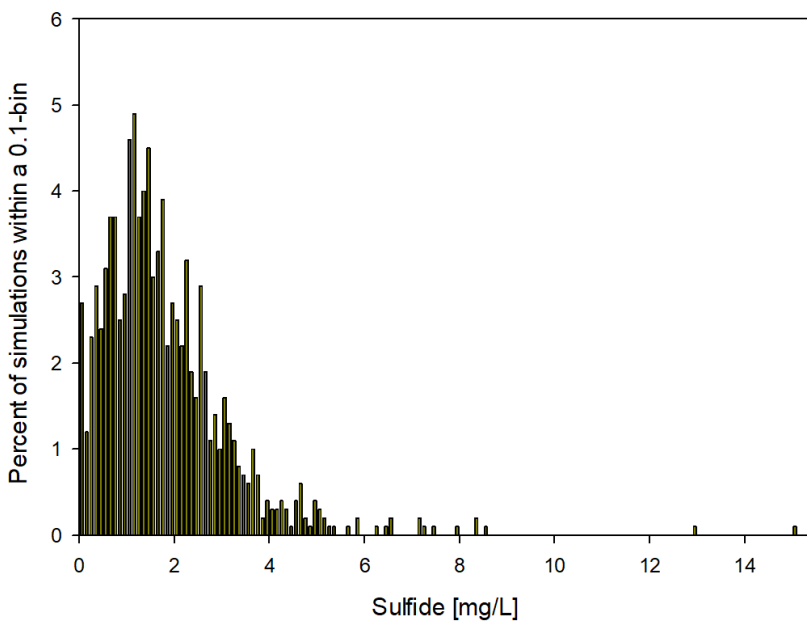


Figure 148. An example of the outcome of a Monte Carlo Simulation varying many parameters as per Mega-WATS default; 1,000 runs

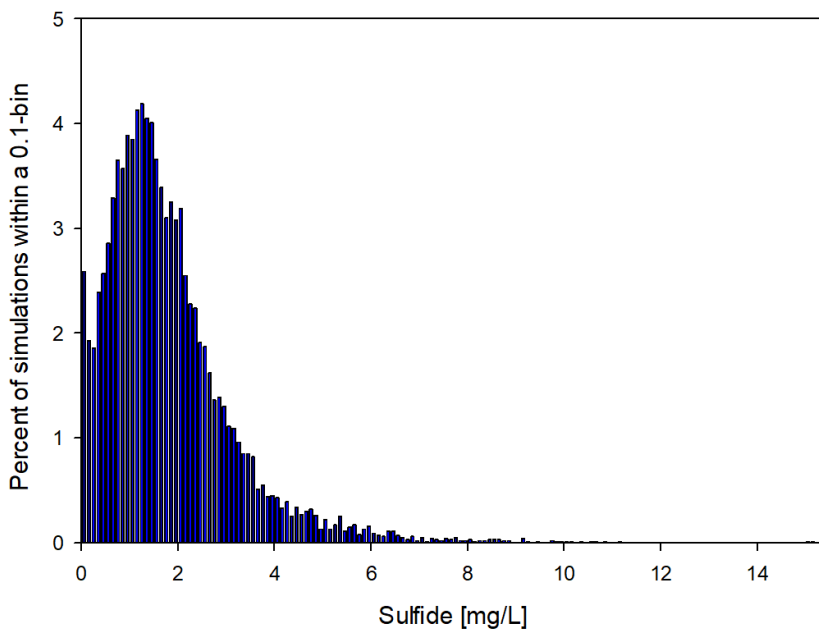


Figure 149. An example of the outcome of a Monte Carlo Simulation varying many parameters as per Mega-WATS default; 10,000 runs

#### 11.4 Running a stochastic simulation

A stochastic simulation is run by pushing the *Run stochastic* button on the main form (lower right corner, Figure 1). This opens the menu shown in Figure 149. If simply pressing *Run*, a message pops up saying that output parameters must be chosen before the stochastic modelling. Once that is done, Mega-WATS remembers the choices for the next run, or they can be loaded the *Load dataset* button.

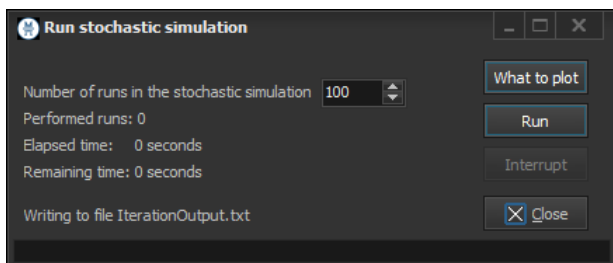


Figure 150. Menu for running stochastic simulations

##### 11.4.1 Choosing output parameters for stochastic modelling

Parameters for stochastic output can be set by pressing the button *What to plot* in Figure 149. The same form (Figure 150) can be accessed via the main form menu *Output* → *What to plot Stochastic*.

Selecting a stochastic simulation output point:

- Chose a pipe. The easiest way is to choose a pipe on the map of the main form and then press the *Chose the selected pipe* button in the top middle of the form.
- Chose where in the pipe to present the stochastic simulation output by sliding the ruler in the top right part of the form.
- Chose which output(s) to show. There are 28 options which can be checked
- Finally press the *Save this plot point* button and a string with pipe name, position, and code for what to plot is shown in the list below the checkboxes.

A single line can be deleted by selecting it and pressing *Clear this plot point*.

Pressing the button *Clear all plot points* will clear all selected points.

Upon pressing the *OK* button, a save dialog appears where the selected points can be saved to. This can also be achieved by pressing the *Save dataset* from the lower right part of the form. Saved datasets can be loaded via the *Load dataset* button.

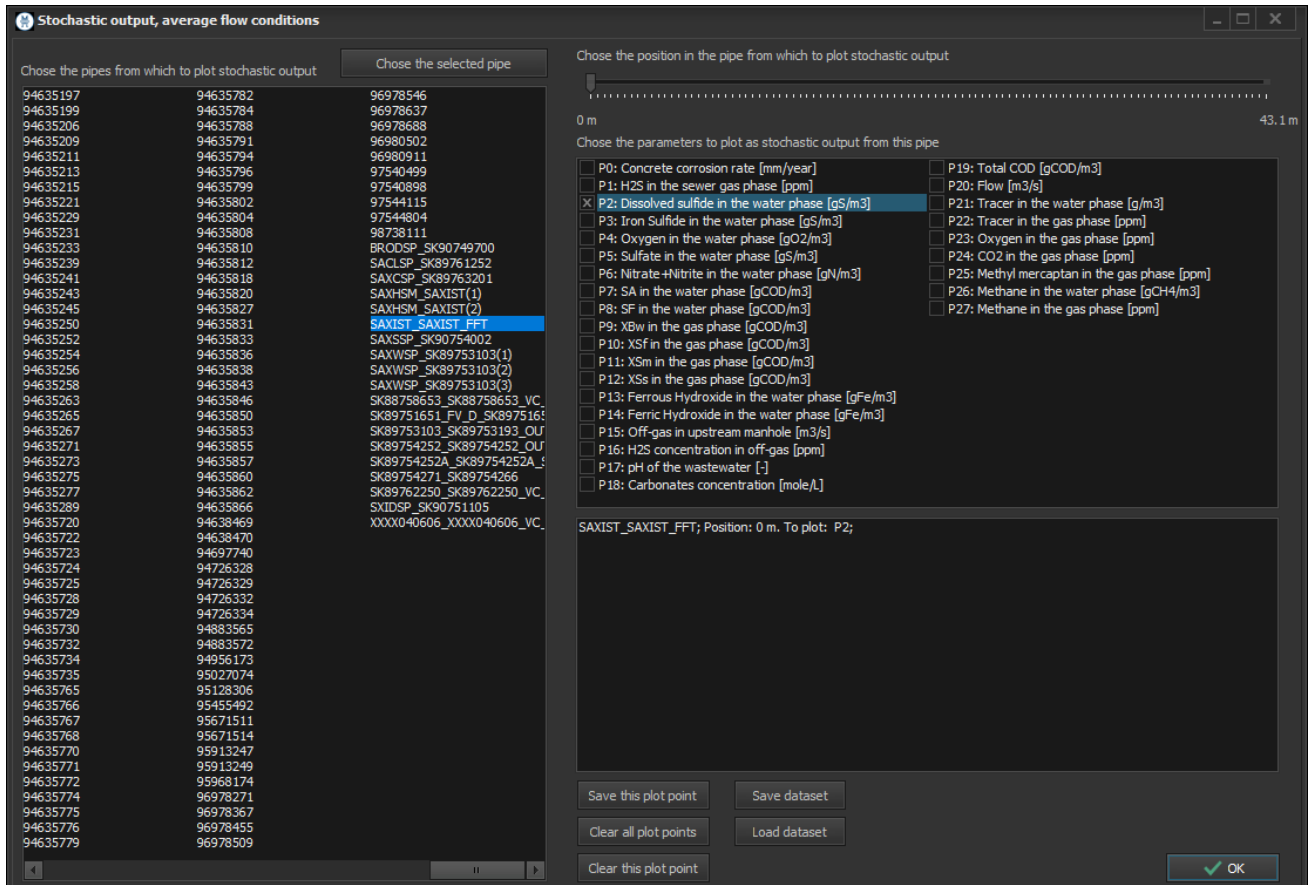


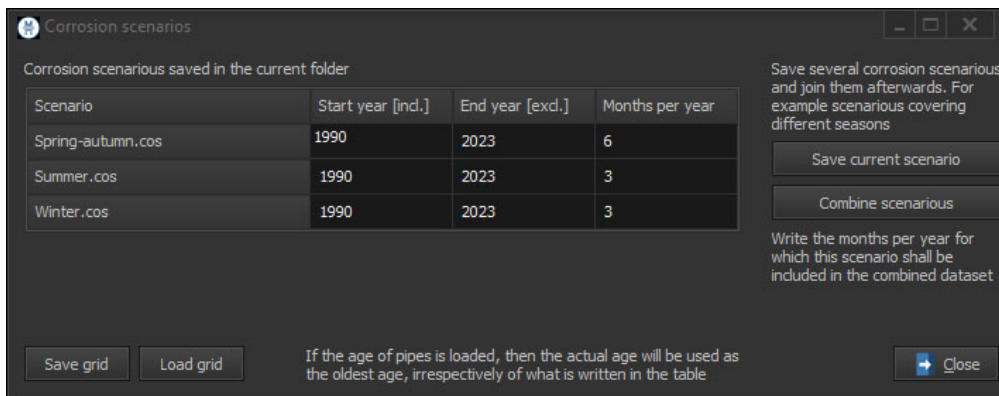
Figure 151. Choosing parameters for stochastic output

### 11.4.2 Running the simulations

Finally, click *Run* in Figure 149. A file *IterationOutput.txt* is created in the directory where the project is stored. It holds all selected output data in a Tab-separated text file.

## 12 Combining corrosion scenarios

Corrosion rates can be combined for multiple scenarios. For example (but not limited to) seasonal variation in the corrosion. This is done as follows: Run the first scenario then open *Tools -> Corrosion scenarios* menu and add the scenario using the *Save current scenario* button. Repeat this for any number of scenarios. Next time the *Corrosion scenario* form is opened, it will list the scenarios saved in the folder where the project is stored. Add a start and end year for the corrosion and a duration per year of that period. This can be saved using the *Save grid* button and loaded again using the *Load grid* button (Figure 151).



Corrosion scenarios saved in the current folder

Scenario	Start year [incl.]	End year [excl.]	Months per year
Spring-autumn.cos	1990	2023	6
Summer.cos	1990	2023	3
Winter.cos	1990	2023	3

Save several corrosion scenarios and join them afterwards. For example scenarios covering different seasons

Save current scenario

Combine scenarios

Write the months per year for which this scenario shall be included in the combined dataset

Save grid Load grid

If the age of pipes is loaded, then the actual age will be used as the oldest age, irrespectively of what is written in the table

Close

Figure 152. Corrosion scenario form allowing combining simulation of various scenarios

The scenarios can now be combined (*Combine scenario* button) using the weights represented by the time each scenario is valid. This overwrites the modeled corrosion rate of the last simulation, and the average corrosion rate can be visualized using the various tools in Mega-WATS. In case pipe age is included, the average corrosion is used for predicting average remaining life and loss of pipe wall thickness. The use of such combination is illustrated in Figure 152, where the scenarios and their time-based weight is used to combine corrosion in different seasons to one corrosion rate.

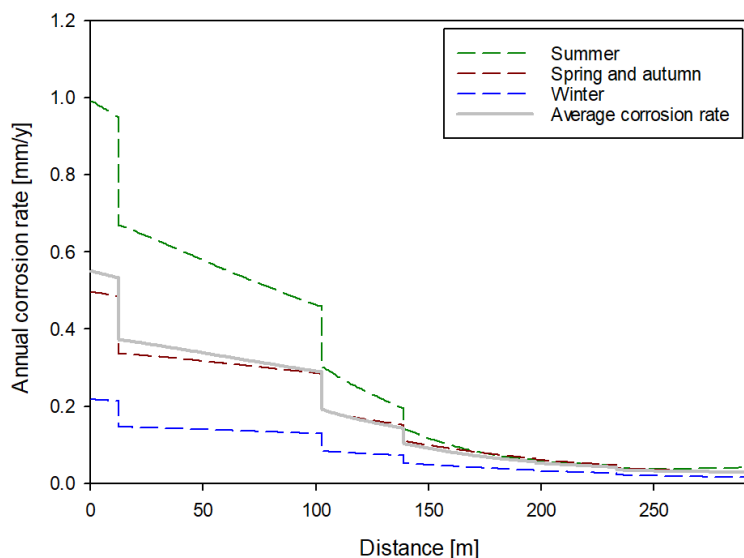


Figure 153. An example of combining corrosion scenarios using the time weights of Figure 151

Note: The simulated corrosion is average rates around the pipe perimeter above the water line. Corrosion is however not homogeneously distributed but tends to be higher at the crown and close to the water line. The actual corrosion rate is hence a factor times the so-simulated rate (Section 7.2).

## 13 Mega-Vent

### 13.1 Air flow simulation

Mega-WATS generates air flow in the pipes by balancing the drag of the water and the friction on the pipe wall (Figure 153).

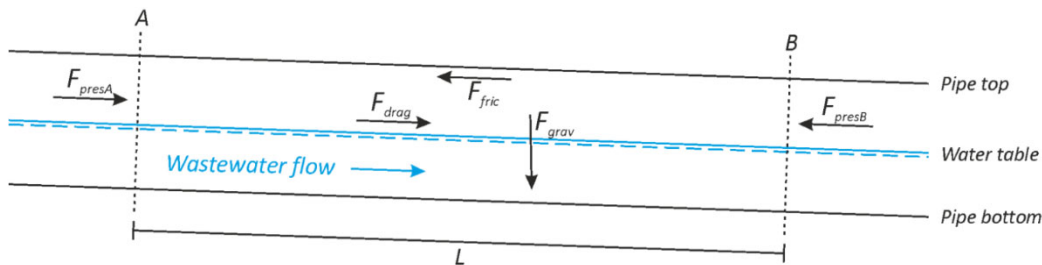


Figure 154. Drag and friction in a sewer pipe

If two connected pipes have different hydraulic characteristics, such as slope, roughness, diameter, shape, etc., the drag and friction will be different. This leads to one pipe having more air flow capacity than the other. In Mega-WATS, the difference is ejected or taken in, depending on the air flow capacity (Figure 154). In other words, the nodes (manholes) are treated as being fully open to the urban atmosphere.

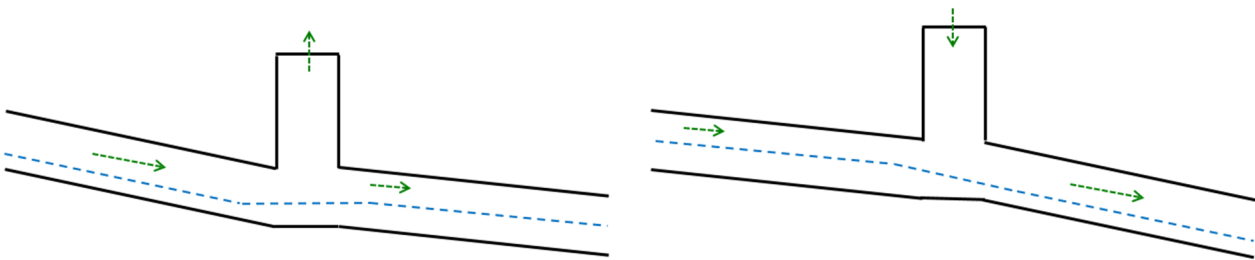


Figure 155. Difference in air transport capacity between two connected pipes

In reality, most sewers are somewhat open to the urban atmosphere, but not unrestrictedly so. A manhole cover has for example pick-holes allowing air in and out but is not fully open. This leads to pressure differences in the sewer, where the actual inflow and outflow of air is governed by the pressure difference between sewer and ambient atmosphere and by the size, shape, and elevation of the openings. This again leads to most sewers exchanging less air than what Mega-WATS predicts.

The issue of Mega-WATS having a simplified approach to air flow in the network is handled by integration with Mega-Vent. The latter is a model that predicts air flow and pressure in sewers. It is a stand-alone model, which can be called, and the simulation results incorporated in Mega-WATS.

Mega-Vent is a sewer ventilation model which represents air pressure, flow, and out/in-gassing within sewer headspaces. Mega-Vent was developed by The WATS Guys, Inc. to augment their ability to do sewer odor and corrosion control analysis by providing the following:

- Accurate headspace air flow values needed as inputs to Mega-WATS
- Prediction of air in/out-gassing under natural ventilation conditions
- Prediction of air reduction at vents due to wind
- Prediction of the vacuum 'zone of influence' resulting from forced ventilation
- Estimation of fan sizing needed to achieve a given zone of influence
- In conjunction with Mega-WATS, estimation of odor loading to scrubber equipment



Mega-Vent builds on the work of Ward et al. (2011a; 2011b), in which ventilation in a partially full flowing pipe was posited as a force balance on the air within each pipe, and Bentzen et al. (2016), in which the coefficients needed to describe drag at the air-water interface were determined experimentally. Forces acting on each air headspace in a pipe network include friction between the moving air and the un-submerged pipe surface, drag between the flowing water surface and air pressure at each boundary, and gravity acting on the mass of air. Following conservation of momentum, the sum of forces equals the time-rate of change in momentum in the air mass in each pipe. Figure 155 illustrates this concept.

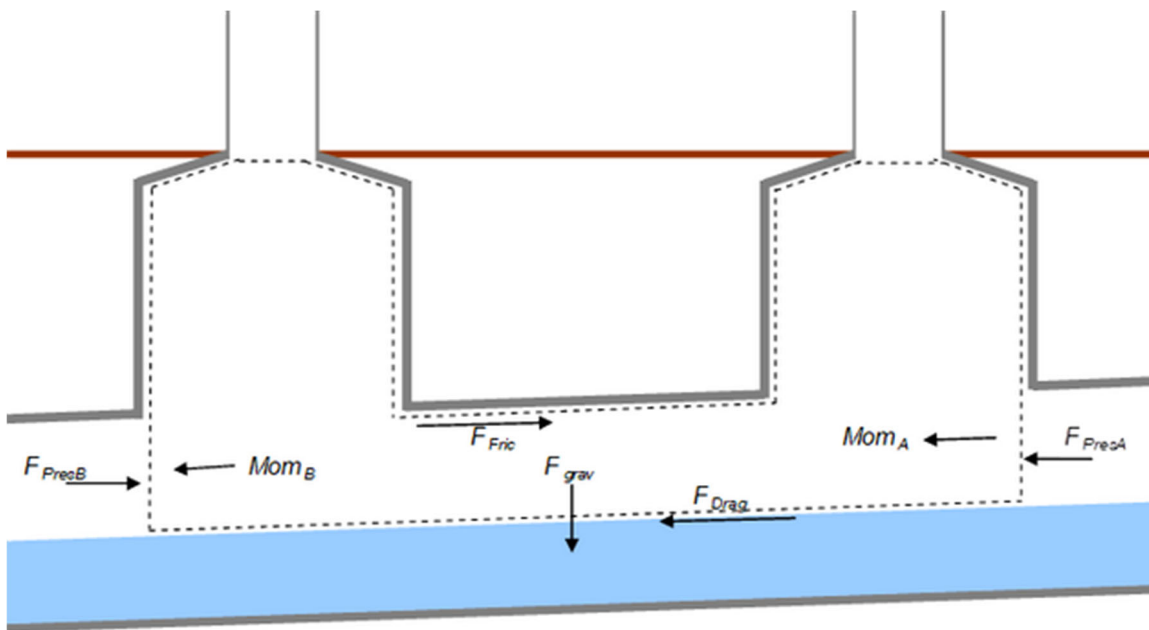


Figure 156. Momentum Balance on the Air in a Partially Full Pipe

Mega-Vent can be implemented over a branched sewer network containing pipes with inter-connected headspaces. It represents air static pressure (relative to ambient pressure) at each node between pipes, air flow in each pipe, and air in/out gassing at each node. Boundary conditions are an important part of the sewer ventilation model and must be specified in terms of the size/shape of openings between the sewer headspace and ambient air and at connections to sewer structures outside the model domain. Air out/in gassing at openings is calculated using discharge equations appropriate to the size/shape of the opening, e.g., sharp-edged orifice. Figure 156 shows a diagram of a simple branched network of three pipes with boundaries to the ambient atmosphere. In Mega-Vent this concept is generalized to any configuration of connected pipes.

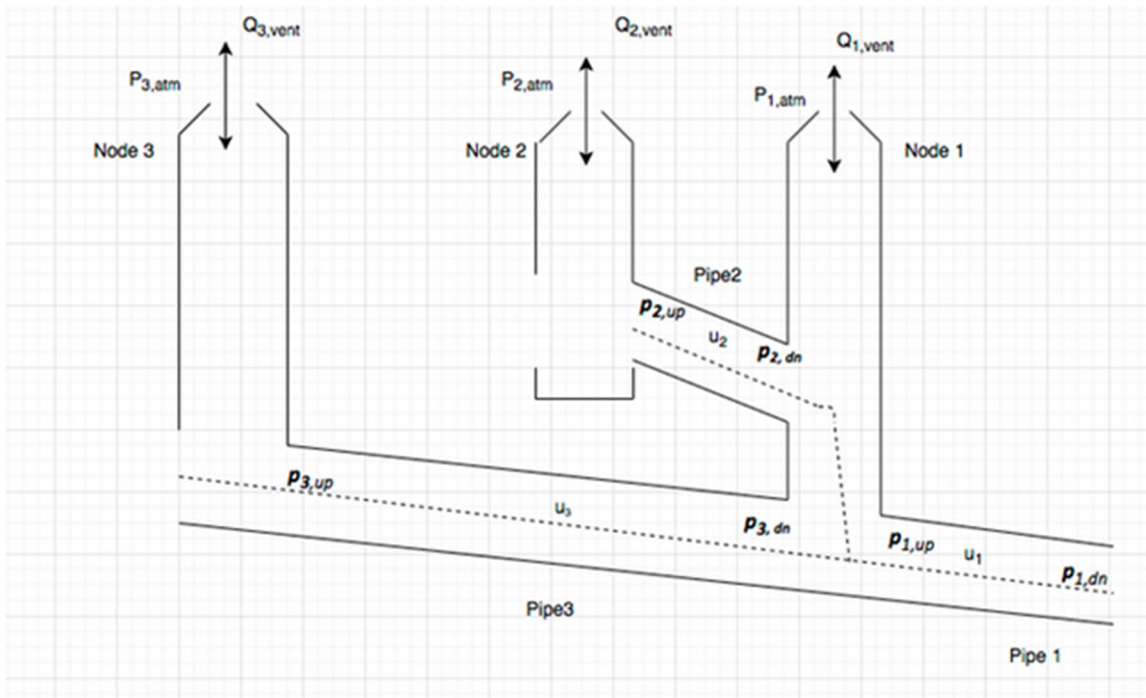


Figure 157. Branched Network Diagram

Inputs to Mega-Vent include pipe physical geometry, water depth and velocity, configuration of vents, and conditions at connections to sewer headspaces outside the model domain. In practice, conditions at connections to sewer components outside the model domain are not easy to know without including those outside components in the model domain – often this is not feasible to do. Instead, field pressure monitoring should be done to obtain information on outside forces bearing on the model domain. The siting, number, and duration of pressure monitoring locations depends on the specifics of the model domain and goals of the project. Pressure monitoring is relatively simple to accomplish using instruments which are robust and inexpensively available for rental. Also, pressure monitoring for Mega-Vent is easily added as part of a field sampling campaign to gather inputs for Mega-WATS.

Ventilation modelling can be completed to characterize gas flow and pressure in the sewer headspace as driven by several relevant forces. These include friction at the air/water interface, forced ventilation by fans, and air entrainment in drop structures. The former two forces can be considered explicitly in terms of force balances on each pipe headspace using a network solution of all connected headspaces. Location and power of fans can be varied to arrive at the optimal amount of forced ventilation needed to prevent fugitive emission over the range of expected flow conditions. That is, the minimum air treatment needed to achieve a consistent vacuum within the tunnel headspace. The resulting headspace ventilation values can then be used in Mega-WATS to inform the odor concentrations that must be treated at the recommended force ventilation facilities. Forces related to plunge-pipe drop structures are treated according to the work of Ma et al (2016), in which air pressure gradients were measured along the height of a plunge pipe drop structure using various flow rates, and a mechanistic model was developed to predict the pressure/ventilation influence of plunge-pipe drops. Research is underway to quantify the pressure/ventilation influence of vortex drop structures. At present, vortex drops are not yet treatable by mathematical models. Therefore, information from physical models (previously completed for other projects) of similar configuration must be adapted as appropriate. It is assumed that waterfall-type drop structures have no net influence on air

pressure/ventilation. This assumption is valid in configurations where air accelerated by the falling water recirculates bottom-to-top without constraint.

## 13.2 Setting up Mega-Vent

Mega-Vent can run in the cloud (Amazon Web Services) or locally on computer where Mega-WATS is installed.

### 13.2.1 Cloud computing

Mega-Vent runs in the cloud in a Linux environment. It is deployed in AWS (Amazon Web Services) and simulations can be executed via calls to REST APIs. It is therefore needed to install Linux shell as follows:

1. Create folders for Mega-Vent files
  - a. Create a new folder `gvm_model` with 2 sub-folders: “input” and “output”, for example `c:\gvm_model`, `c:\gvm_model\input` and `c:\gvm_model\output`
  - b. In `c:\gvm_model\input` you will place the input files and
  - c. In `c:\gvm_model\output` the script will download the results from the runs
  - d. Copy the `gvm_exec2.sh` to the folder `c:\gvm_model`.
2. Perform this step for Windows systems only. Follow the directions from <https://www.howtogeek.com/249966/how-to-install-and-use-the-linux-bash-shell-on-windows-10/> to install the bash shell.
  - a. Enable the Windows Subsystem for Linux and reboot Windows.
  - b. Install Ubuntu from windows store

Upon having installed the shell, Mega-Vent can be called from Mega-WATS.

### 13.2.2 Local computing

The local version of Mega-Vent can be obtained on request from The WATS Guys in case the user experiences issues getting the cloud computing to work, for example due to IT security issues.

Unpack the zip-file into a folder, for example a subfolder called `gvm_main` under the Mega-Vent root directory (e.g., `c:\gvm_model\gvm_main`).

Uncheck the checkbox *Use cloud computing (bash)* and make sure that the directory shown to the right of the button Local Mega-Vent directory is the correct directory.

For the local version of Mega-Vent, input and output directories can be chosen freely.

## 13.3 Calling Mega-Vent

On the right-hand side of the Mega-WATS graphical user interface, chose ‘Page C’ (Figure 4). Then click the button ‘Mega-Vent integration’ and the menu shown in Figure 157 shows up.

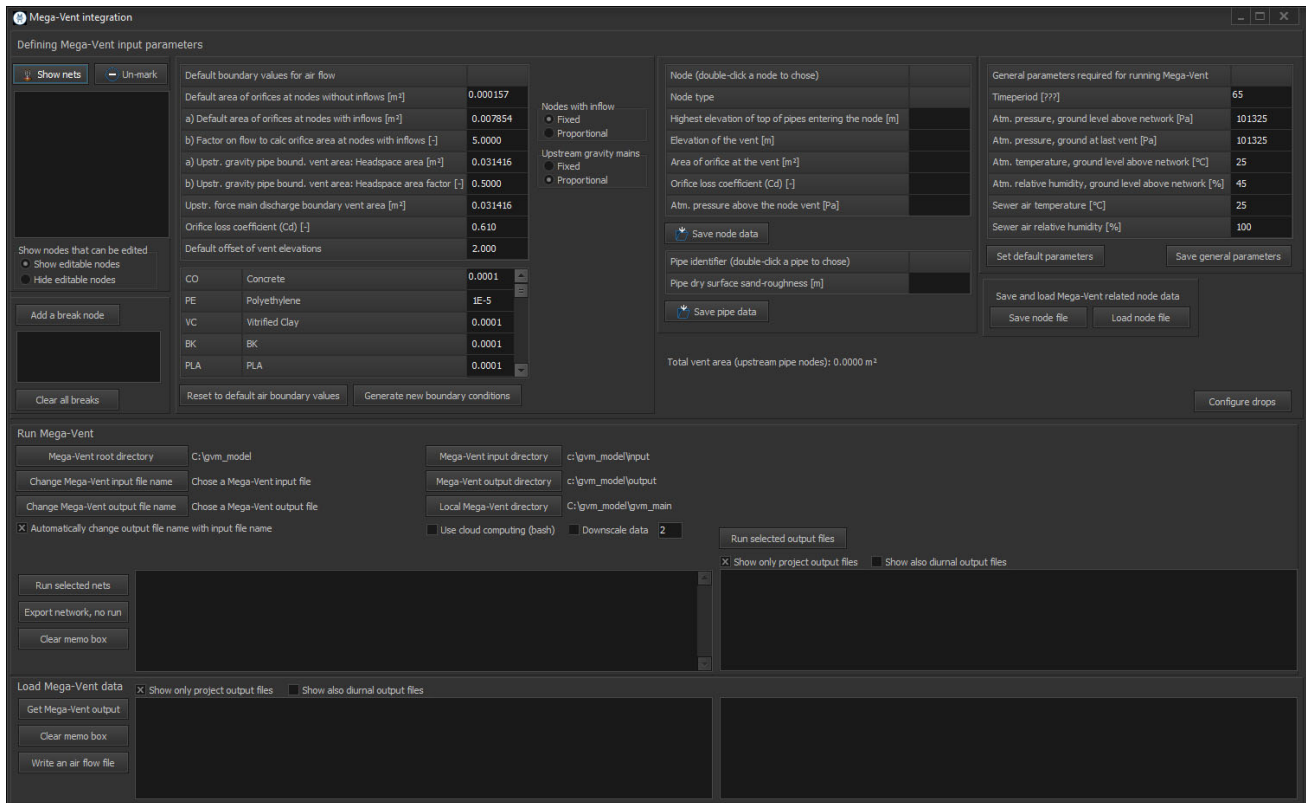


Figure 158. Mega-Vent integration menu

First press the button ‘Show air flow nets’, which shows the networks separated by zones (region of contiguous headspace). For example, when two parts of the network are connected by force mains, this means that water can flow but not air. The same goes if there are syphons or pipes running full for other reasons. These air networks are hence pneumatically separate and simulated separately in Mega-Vent. The output from Mega-Vent is then stitched together into a Mega-WATS air flow file for the whole network.

### 13.3.1 The different node types

Figure 158 shows one such air flow net after selecting in the Mega-Vent integration menu. The net holds 393 pipes. The nodes in the Mega-WATS interface have different colors depending on node characteristics. The light blue nodes, for example, are nodes receiving inflow while the grey ones are nodes without inflow and without any other special characteristics. The full list of nodes and their color coding is given in Table 10.

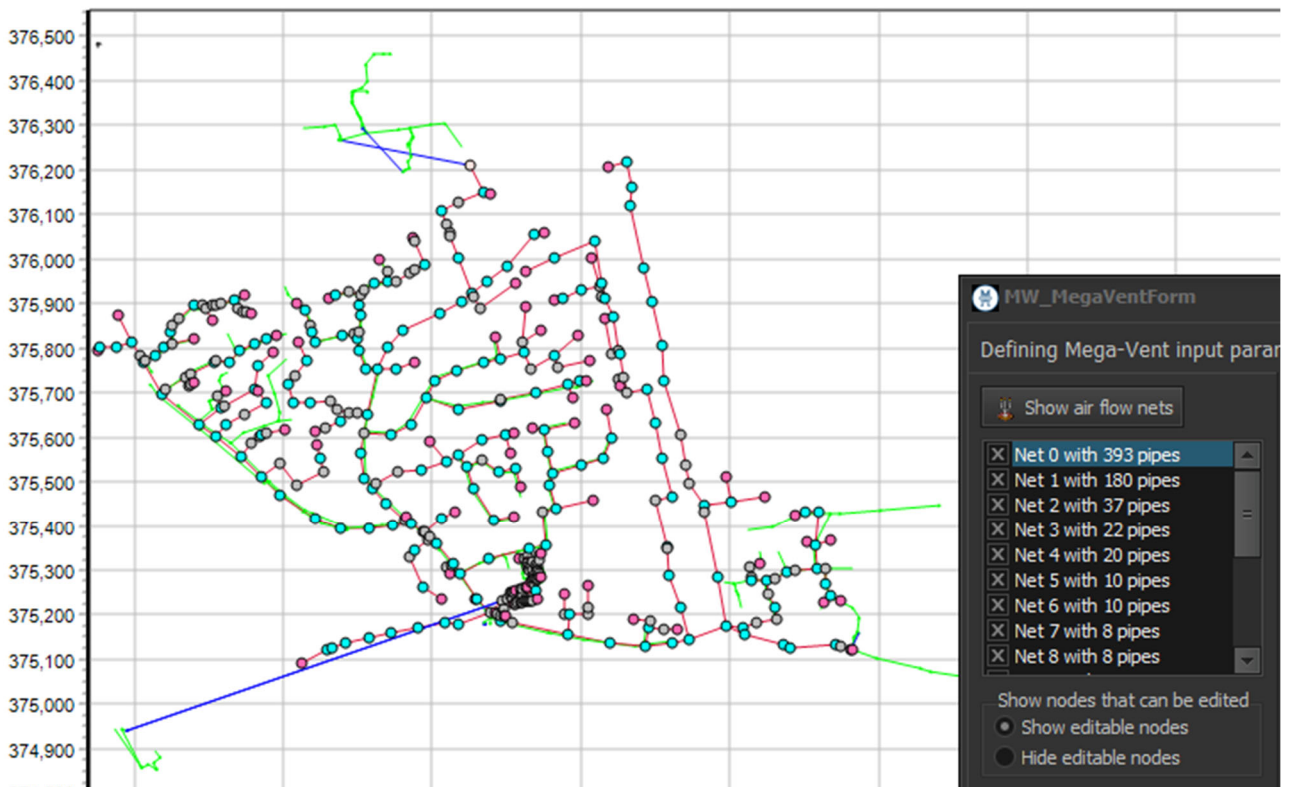









Figure 159. An example of an air flow net

Table 10. Coloring of nodes for Mega-Vent setup

Node	Color	Description
	Grey	Standard node. The node has no special characteristics. It is assumed it is only ventilated by pick holes in the manhole cover
	Aqua-blue	Node with inflow. When a node has inflow, it is assumed that there is a connecting pipe not included in the model domain. Sometimes it can be inferred that these nodes are ventilated at house level, for example by roof top ventilation. Otherwise, ventilation may be inferred from the size of the water inflow.
	Hot-pink	Upstream boundary node connected to pipes not included in the model domain.
	Misty-rose	Force main discharge to gravity system. No upstream gravity pipe. Because force mains flow full, these nodes represent upstream air locks (except if they are vented at street level)
	Blue	Network discharge node – downstream-most node
	Yellow	Node that has been edited
	Black	Node inserted to break the network. These are designated manually to eliminate sections of an air net from the model domain.

### 13.3.2 Default settings of node characteristics

The default setting for ventilation of all nodes is shown in the default boundary table (Figure 159).

- a) The default cross-sectional open area of a street-level vent (orifice) at a node without special characteristics and without inflow is set based on what is known about the type of manholes used in the network. For example, lids with four pick holes may have a total open area of 4 cm<sup>2</sup>. In other networks where manholes are sealed with gaskets, there is effectively no street level vent and the default orifice area should be set at a very small, non-zero value: for example, 0.0001 cm<sup>2</sup>. As default, the vent area is set to the area of two circular pickholes of 1 cm diameter each.
- b) The default area of an orifice at a node with inflow represents a boundary connection to a pipe not included in the model domain, i.e., not a street-level vent. How large not-included pipes are and how they terminate at their upstream ends must be inferred by the context of the network or other information, such as GIS or as-built drawings. However, it is reasonable to assume they are no larger than the largest pipe not included in the hydraulic model. For example, if the air network is based on a hydraulic model which included all gravity pipes 30 cm and larger, then the connecting pipe must be 25 cm or smaller. So, the upper bound on the size of the connecting pipe is 25 cm and the lower bound is 10 cm (assuming upstream roof vents have a diameter of 10 cm). Selection of the default orifice size should also allow for the fact that the connecting pipe is not open to the atmosphere but has some indirect connection to the atmosphere through roof vents, etc. The default assumption in Mega-WATS is that it has an orifice of 10 cm.
- c) When working with a simplified network such as an interceptor excluding branches, scaling the orifice size based on the size of the incoming flow may be more appropriate – large flows are not delivered by small pipes. The user can choose between the default area option and the scaled-to-flow option by setting the radio button ‘nodes with inflow’. The area is calculated as a factor times the inflow (e.g., 5 s/m × 0.001 m<sup>3</sup>/s = 0.005 m<sup>2</sup>).
- d) Upstream gravity pipe boundaries usually represent the upstream extent of the hydraulic model, and it can be assumed that the not-included connecting pipe is the largest excluded size. For example, if the hydraulic model included all pipes 30 cm and larger, then the connecting pipe is likely 25 cm, and the default orifice size may be selected as one half of the open headspace of a 25 cm pipe. The area is calculated as the sum of the headspace area of the pipes exiting the nodes multiplied by a factor. Mega-WATS suggests a default factor of 0.5.
- e) Upstream force main discharge boundaries should be assumed to be fully closed since they flow full. The orifice size then should be selected to represent the street-level vent. This may be a pick hole or a goose-neck vent or some other structure such as a hatch with a small crack around its perimeter. Lacking any information on the street level vent, the orifice area assumption for these nodes should be the same as for nodes without special characteristics as discussed, i.e., pickhole, etc.
- f) All orifices are simulated by orifice discharge equations which use a discharge coefficient. The discharge coefficient depends on its shape, for example, sharp edged, rounded, etc. A good default is 0.61 which corresponds to sharp-edged or square shoulder, thin plate orifices.

The orifice discharge coefficient is analogous to the minor loss coefficients relating to discharge through duct fittings. For this reason, equivalent orifice discharge coefficients may be selected for gooseneck vents, stacks, and other structures that are not actually orifices. This equivalence is given as follows:

$$C_d = (1/K)^{0.5}$$

Where  $C_d$  is the equivalent orifice discharge coefficient of a non-orifice vent, and  $K$  is the sum of minor loss coefficients in the vent structure. For example, a 10 cm gooseneck vent has a sharp



- entrance, bend, and exit and  $K$  equals  $1 + 0.2 + 1 = 2.2$ . Representing the vent as a 10 cm orifice, the equivalent  $C_d = (1/2.2)^{0.5} = 0.67$
- g) All orifices have an elevation. The default is 2 m above the pipe top. Treatment of buoyancy forces is under development but is not currently included. Until buoyancy forces are included, vent elevation does not matter.
  - h) The atmospheric pressure outside of each orifice, compared to the calculated pressure inside the orifice gives the driving force for air discharging through the orifice. The default is set to the network-wide atmospheric pressure, e.g., 101,325 Pa, or whatever is the typical atmospheric pressure of the city in question. If wind is being simulated, then the Bernoulli equation can be used to select a lower-than-average atmospheric pressure corresponding to wind speed.
  - i) Each pipe has an equivalent sand roughness pertaining to the friction of air flowing across the unsubmerged pipe surface. This roughness is linked to the pipe material and can be set individually per material used in the network.

Default node and pipe values can be changed by changing the values in the tables, then pressing the button “Generate new boundary conditions” (Figure 159). Note that this must be done before changing individual nodes, as this operation will over-write all changes made.

Default boundary values for air flow		
Default area of orifices at nodes without inflows [m <sup>2</sup> ]		0.00040
Either: Default area of orifices at nodes with inflows [m <sup>2</sup> ]		0.00400
Or: Factor on flow to calc orifice area at nodes with inflows [-]		10.00
Upstr. gravity pipe bound. vent area: Headspace area factor [-]		0.3500
Upstr. force main discharge boundary vent area [m <sup>2</sup> ]		0.1000
Orifice loss coefficient (Cd) [-]		0.610
Default offset of vent elevations		2.000
Atmospheric pressure above the vent [Pa]		101325
Nodes with inflow		
<input type="radio"/> Fixed area <input checked="" type="radio"/> Flow proportional area		
CO	Concrete	0.0005
VC	Vitrified Clay	0.0001
BK	BK	0.001
PLA	PLA	0.0001
Plast	Plast	0.0001
Reset to default air boundary values		Generate new boundary conditions

Figure 160. Default node boundary values for ventilation simulation

### 13.3.3 Changing settings of individual nodes

A node can be selected by double-clicking it. This causes the node characteristics table to be populated (Figure 160). Sometimes (when many pipes enter a node) it can be difficult to select a node by this approach. In such case one can double-click on the upstream or downstream node name in the pipe data list-box (Figure 6), which also causes this node to become selected for editing.



Node: JNT_83800826	
Node with inflow	
Highest elevation of top of pipes entering the node [m]	6.494
Elevation of the vent [m]	8.494
Area of orifice at the vent [m <sup>2</sup> ]	0.0000800
Orifice loss coefficient (Cd) [-]	0.650
Atmospheric pressure above the node vent [Pa]	101325
<input type="button" value="Save node data"/>	

Figure 161. Node characteristics table

Individual node values can be changed manually by first selecting a node (Section 13.3.1), then changing the values in the table (Figure 160). Finally press ‘Save node data’ to store the changes.

#### 13.3.4 Forced ventilation

All nodes have a pressure above them. This value is changed in ‘Atmospheric pressure above the node vent’ of Figure 160. Most nodes will have the default atmospheric pressure assigned here. However, if a node has forced ventilation by means of a fan, setting this value to a value below the default atmospheric pressure will simulate a fan extracting air from the system. Setting it below the default atmospheric pressure will create a place where air is actively sucked out of the network. Note that forced ventilation involves connecting a duct pickup, so the vent area also should be revised to reflect the size of the pick-up duct.

#### 13.3.5 Changing roughness of a pipe

As discussed in section 13.3.2, the roughness of a pipe above the water line is used in the Mega-Vent simulations. To change the default value, first select a pipe by double-clicking it on the map, then change the value and save the pipe data (Figure 161).

Pipe: 50516945	
Pipe dry surface sand-roughness [m]	0.000600
<input type="button" value="Save pipe data"/>	

Figure 162. Pipe characteristics table

#### 13.3.6 Global Mega-Vent parameters

Mega-Vent needs several global parameters, namely:

- a) Time period (not currently in use)
- b) Atmospheric pressure at the ground level above the network
- c) Atmospheric pressure at the last node of the network
- d) Atmosphere temperature at the ground above the network
- e) Atmosphere relative humidity at the ground above the network
- f) Sewer air temperature
- g) Sewer air relative humidity

These values are set in the global parameters table (Figure 162).

General parameters required for running Mega-Vent	
Timeperiod [???	65
Atmospheric pressure, ground level above network [Pa]	101325
Atmospheric pressure, ground at last vent [Pa]	101325
Atmospheric temperature, ground level above network [°C]	25
Atmospheric relative humidity, ground level above network [%]	45
Sewer air temperature [°C]	25
Sewer air relative humidity [%]	100

Figure 163. Global parameters used in Mega-Vent

### 13.3.7 Configuring the downstream boundary

The downstream most node of an air network is special because it is not assigned an orifice or other structure constraining air entry/exit. The default assumption is that the downstream open area is equal to the dry pipe cross-section. This would be a good assumption, for example, where a pipe ‘day-lights’ into an open channel. More usually, there is some type of structure constraining air exit at the downstream-most node. The user may need to add an artificial pipe, or modified flow depth to the Mega-Vent input file (discussed below) to better constrain the downstream boundary. Note that full-flowing pipes are not included in the air net. Therefore, using a full pipe to constrain the downstream end of an air network won’t work. However, a ‘dummy’ pipe may be added with a flow depth selected to result in an appropriately constricted boundary.

Also affecting the downstream boundary is the atmospheric pressure in the last vent (Figure 162). This value can be assigned to represent the same global atmospheric pressure elsewhere in the network, or to represent a fan.

### 13.3.8 Configuring drop structures

Drop structures assert different drag on the water. The type of drop structure can be modified (Figure 163).

*This part is not yet set up and functional.*

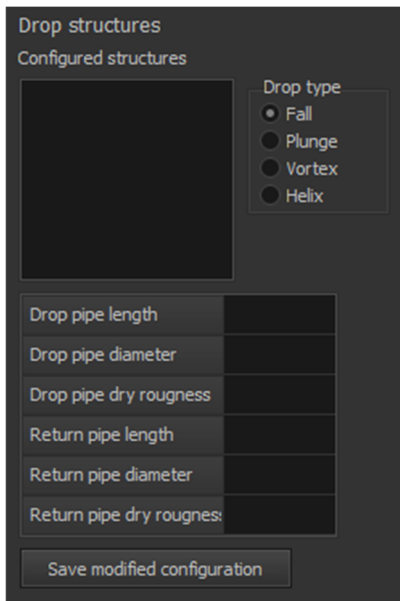


Figure 164. Drop structure configuration parameters

### 13.3.9 Breaking up networks

Mega-Vent can run large networks, but the calculation time increases as network size grows. If the network becomes too big to run in a reasonable time, the network can be broken up and run in pieces. This is done as follows:

- a) Press the 'Add a break node' button (Figure 164)
- b) Double-click a node where the network is to be broken up, the nodes turns black
- c) Repeat a and b till sufficient break nodes have been added
- d) See the broken-up network by clicking 'Show air flow nets' (Figure 158).

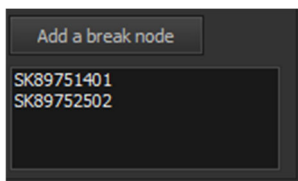


Figure 165. Adding break nodes

A break node can be removed by reversing the process as follows:

- a) Press the 'Add a break node' button (Figure 164)
- b) Double-click a black node where the network was broken up, the nodes turn back to its original color
- c) Repeat a and b till sufficient break nodes have been removed
- d) See the modified network by clicking 'Show air flow nets' (Figure 158).

### 13.3.10 Avoid flow divisions

Mega-Vent cannot handle flow divisions, i.e., when the water splits into two or more downstream pipes. This might cause the Mega-Vent simulation to crash or never complete. Flow divisions can be viewed by checking the *Show flow divisions* ≥ checkbox on Page B of the main form.

### 13.3.11 Choosing directories for Mega-Vent

Data files from Mega-WATS must be stored on the computer before being sent to Mega-Vent. First chose the Mega-Vent root directory previously discussed in Section 13.2 (Figure 165). If the default names stated in that section are used, Mega-WATS identifies the directories automatically.

The user can change the Mega-Vent root directory. When running Mega-Vent in the cloud, the input and output file directories must be placed as subdirectories to the root directory and named input and output, respectively. If Mega-Vent is run locally, the user can freely change all directory names.

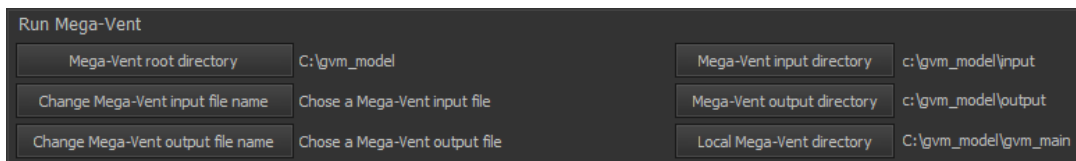


Figure 166. Directories for Mega-Vent

#### 13.3.11.1 No spaces are allowed in Mega-Vent file names

Mega-Vent directories and file names must not contain spaces. If the project name contains spaces, Mega-Vent will substitute those with 'underscore' ( \_ ). If directory names contain spaces, Mega-Vent will not allow those to be chosen.

### 13.3.12 Running Mega-Vent

First select one or several networks in Show nets list-box (upper left corner) (Figure 166). If only one is selected, the buttons *Change Mega-Vent input file name* and *Change Mega-Vent output file name* can be used to rename the files. If several are selected, or if a diurnal flow variation is loaded, Mega-WATS will auto-create file names.

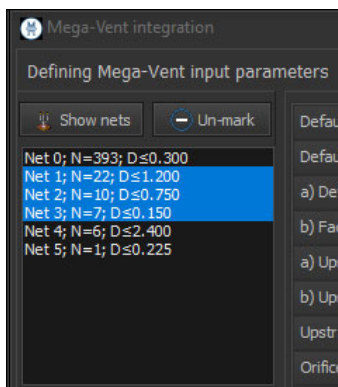


Figure 167. Selecting nets for export and running in Mega-Vent

Either export the network by pressing the *Export network* button and then press *Run selected nets* or by pressing *Run selected nets* directly (Figure 167). The first option is useful if the Mega-Vent input files are to be manually assessed and modified before running.

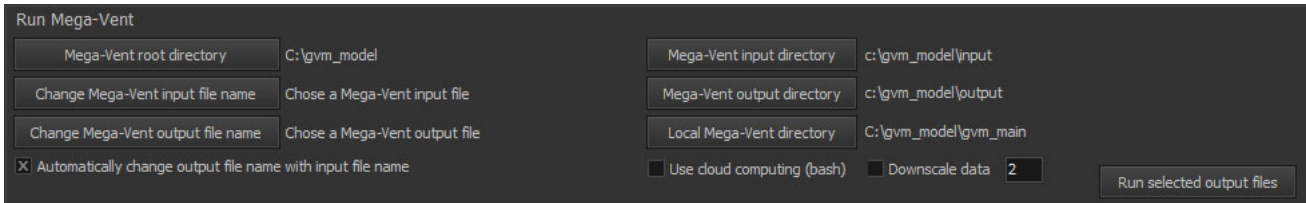


Figure 168. Running Mega-Vent from Mega-WATS

A Mega-Vent command prompt opens showing the progress of each simulation. Depending on the size of the network sent to Mega-Vent, this takes several minutes or more.

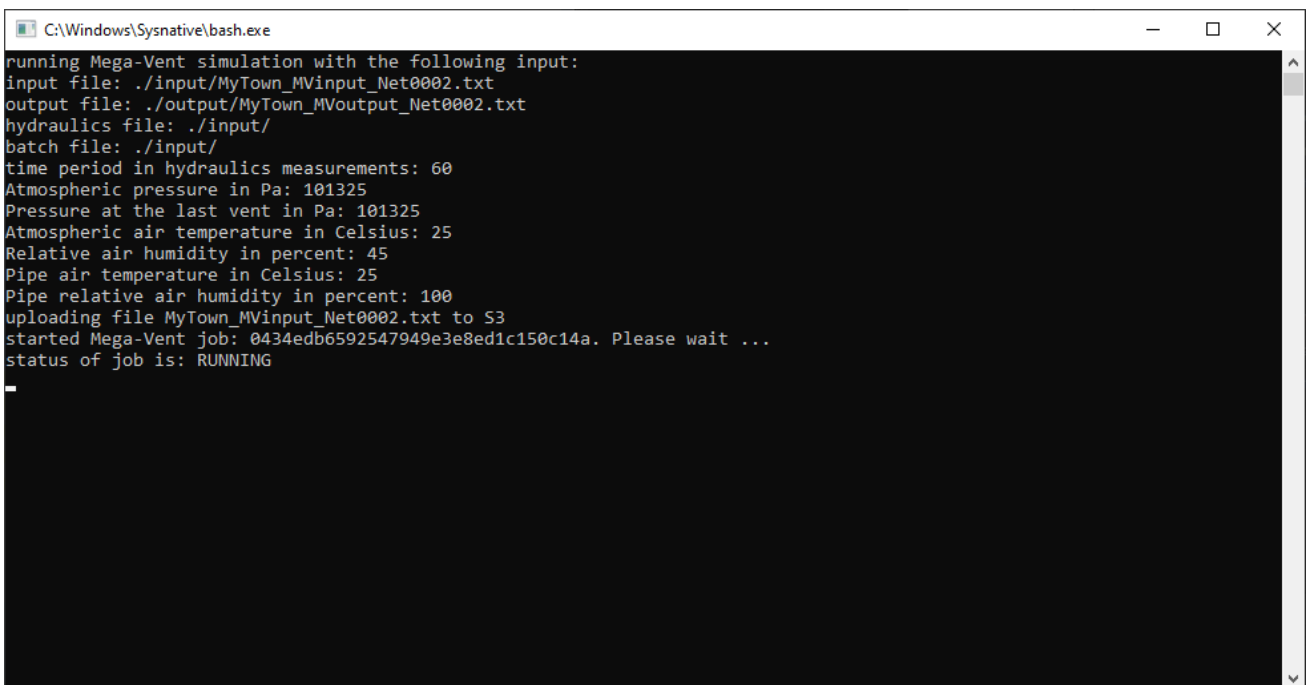


Figure 169. A command prompt running a Mega-Vent simulation in the cloud.

When the process has completed, the bash-shell closes. Closing it manually will cause the Mega-Vent simulation to terminate. The time and description of each process is logged in the windows to the right of the buttons (Figure 169). For example, can it be seen that the job in question was sent to the cloud at 5:01:00 PM and received back at 5:13:31 PM.

The user can run an many jobs in parallel.

Already exported files can be run separately by choosing them in the upper-right list-box of Figure 169 and pressing the *Run selected output files*.

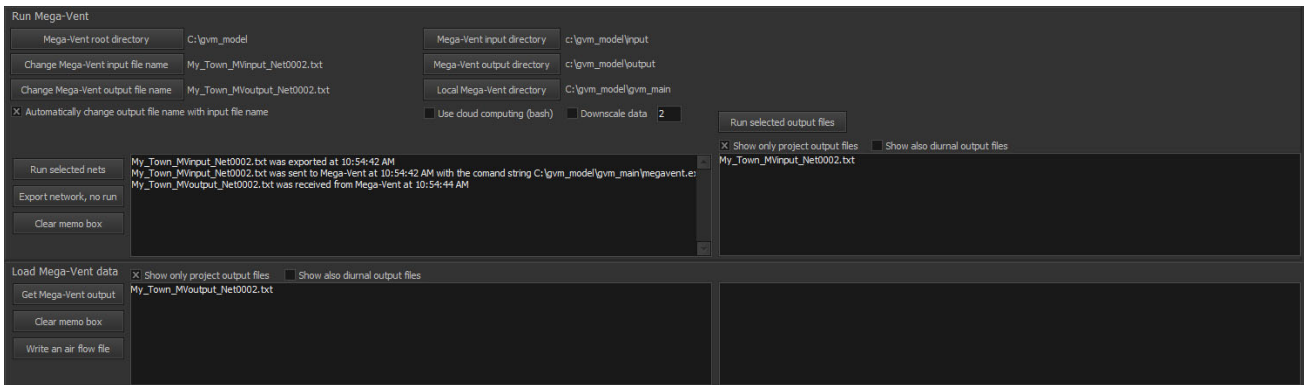


Figure 170. Logging the processes

### 13.3.13 Check if the simulations converge – downscaling

When pipe diameters are large, there is a risk that Mega-Vent does not converge. In such case, Mega-Vent will still complete a run, but the calculated pressure and air flows are meaningless. This can be checked when retrieving Mega-Vent output into Mega-WATS by pressing *Get Mega-Vent output*. Figure 170 shows an example of a simulation which did not converge. It shows that the lowest pressure is  $-1.81850173712 \cdot 10^{16}$  Pa and the highest pressure is 45,623,249.650 Pa. This is obviously impossible and indicates that simulations did not converge.

```
Doha_MVoutput_Net0000.txt loaded - Max error: 0.008663 Mean error: 0.006199 Min pressure: -1.81850173712E016 Max pressure: 45623249.650
```

Figure 171. Text listed in the lower right text output form when retrieving a Mega-Vent simulation which did not converge.

This is fixed by downscaling the pipes and flows by checking the Downscale checkbox and writing an appropriate number in the edit box. Try first with two, if that does not work, then increase to e.g. 4. Continue till the simulations converge like shown in Figure 171, where the pressures now are reasonable. When importing the data, the scaling factor in the edit box must be the same as when sending it, as this is used to scale the diameters and flows back up.

```
Doha_MVoutput_Net0000.txt loaded - Max error: 0.000342 Mean error: 0.000021 Min pressure: 101323.065 Max pressure: 101325.08
```

Figure 172. Text listed in the lower right text output form when retrieving a Mega-Vent simulation which did converge.

### 13.3.14 Running diurnal variations

Mega-Vent can calculate air flow for diurnal flow variations. After having run Mega-WATS with diurnal flow variation, the panel *Run diurnal variations* becomes visible on the Mega-Vent integration form. A time series of Mega-Vent files is created by setting the *From timestep* and *To timestep* spin edits to the desired values (Figure 172) and then pressing the *Run selected nets* button.

If the Mega-Vent files end with *\_dt\_#* (# is the time step), then the file belongs to a time variation (Figure 173). When loading, and if all time steps are not given, or there is no *\_dt\_#* at the end of the file name, then time steps are set equal to the first file loaded for the respective net.

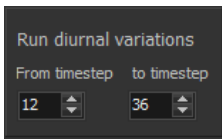


Figure 173. The panel allowing diurnal variations to be sent to Mega-Vent

Do this for one network at a time, not a batch of networks, as the number of windows which can be kept open on a Microsoft Windows machine is limited.

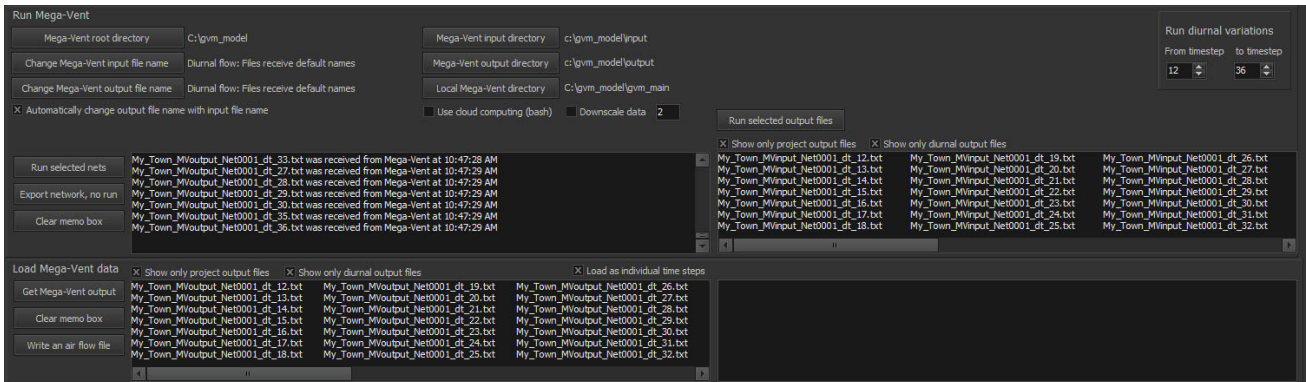


Figure 174. The bottom part of the Mega-Vent integration form after having run a diurnal variation.

### 13.3.15 Loading a Mega-Vent simulation

Finally load the Mega-Vent simulation by pressing 'Get Mega-Vent output' (Figure 169). After having loaded the desired number of Mega-Vent output files, Mega-WATS can be run by pressing the 'Run Once' button on the main form.

The Mega-Vent created data are stored in the network and flow data of Mega-WATS. To create a permanent air flow file, which can be loaded from the 'Build project' form, use the 'Writ an air flow file' button.

### 13.3.16 Showing air flows and pressure in Mega-WATS

Chose page C (Figure 4) to show air flow and pressure. One can chose to visualize air pressure at nodes, air flow in pipes, and air velocity in pipes. Flow rates and velocities are shown by pipes (Figure 174). Blue indicates that the air flows in the same direction as the water (co-current), while pink indicates counter-current air flow. By dragging the drag-bar, the cut-off value changes. By pressing the (+) speed-button, the showing changes between above and below the chosen set-point.

Pressure at nodes can also be visualized (Figure 175).



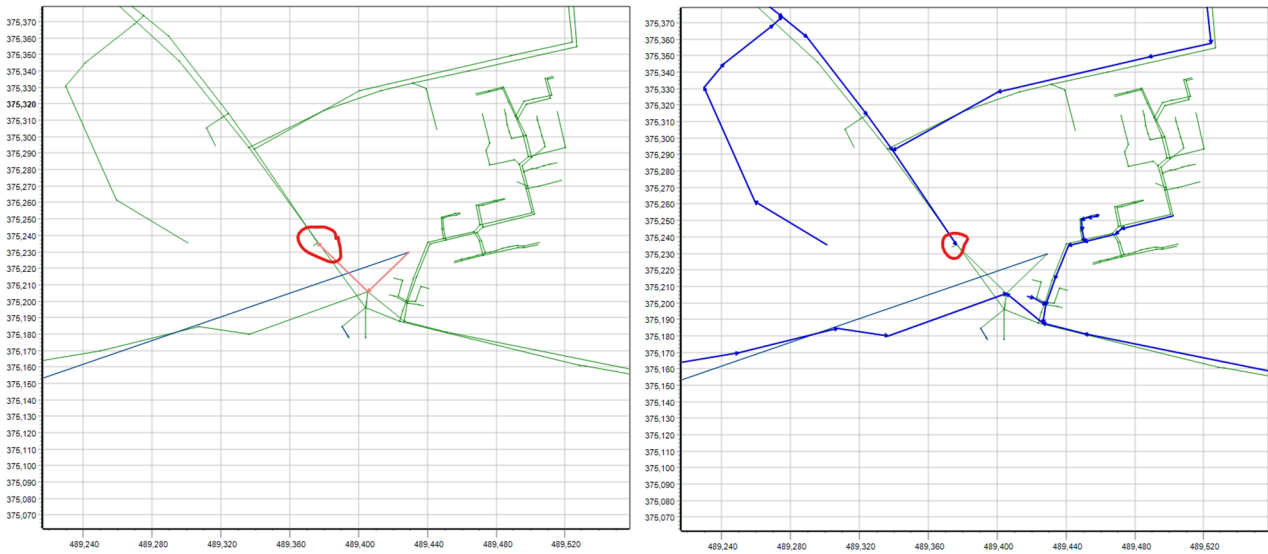


Figure 175. Counter-current (left) and co-current air flow (right) in the pipes. The red markings indicate where a fan is extracting air

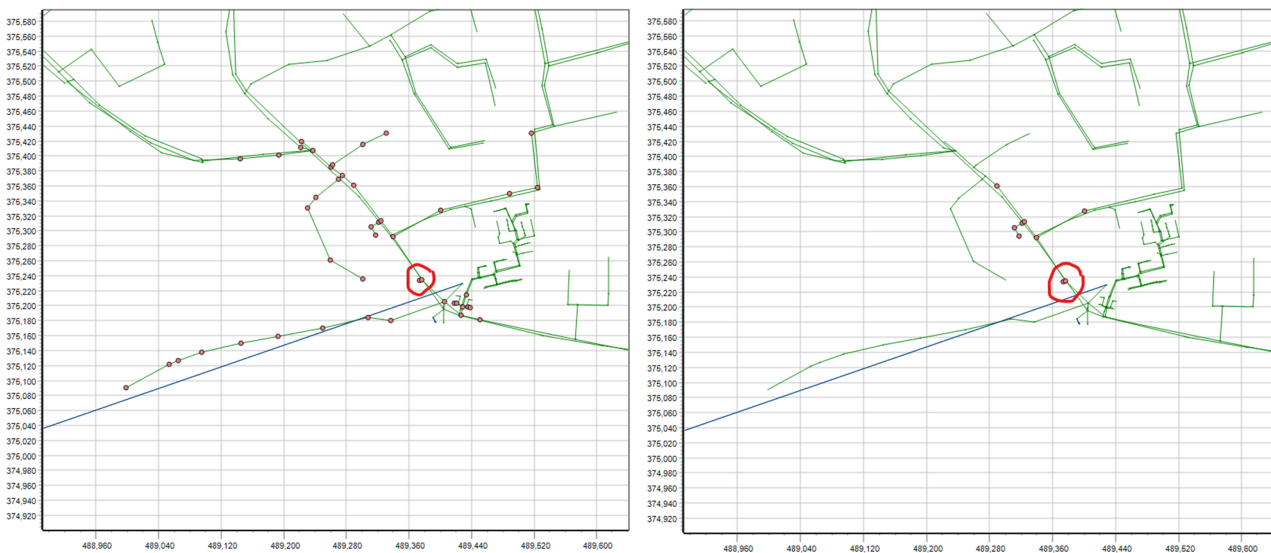


Figure 176. Two different negative pressure levels. The red markings indicate where a fan is extracting air

### 13.4 Air displacement

Mega-Vent does not calculate air displacement when flow is varying over time. If the amount of water in a pipe increases, this will lead to air being pushed out of the system (pressure increase), while air will be pulled in when water levels drop. The pressure generated by these perturbations propagate with the speed of sound and can hence for all practical purposes be treated as instantaneous. If water levels for example rise at the end of a long (closed) tunnel, an increase in pressure will be felt instantaneously at its beginning.

Mega-WATS instead calculates the air displacement according to the varying flow pattern. The view of air displacement is only shown for diurnal simulations, as this is the only case where air displacement can be calculated. It is chosen on the *Physics* tab (Figure 176).

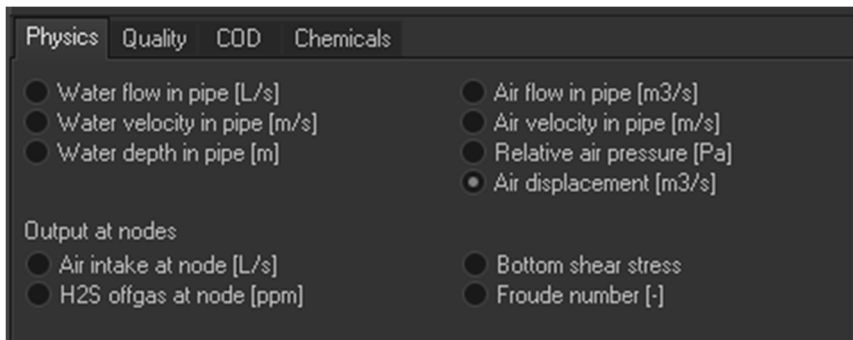


Figure 177. Showing air displacement for diurnal simulations.

An example of a long and large tunnel is shown in Figure 177. The tunnel is approx. 13 km long and of 4.5 m in diameter. It holds in the simulation example on average around 165,000 m<sup>3</sup> of air. The displacement per second maximizes at 4 m<sup>3</sup>/s. Had the tunnel been closed completely airtight, this displacement would have led to a pressure change. However, the tunnel has air dampers at both ends, and the displacement will hence lead to an additional amount of air being pushed out of the tunnel. When assessing odor release, and when assessing the size of a fan controlling the air pressure in the network, this displacement must be added to the values generated by Mega-Vent.

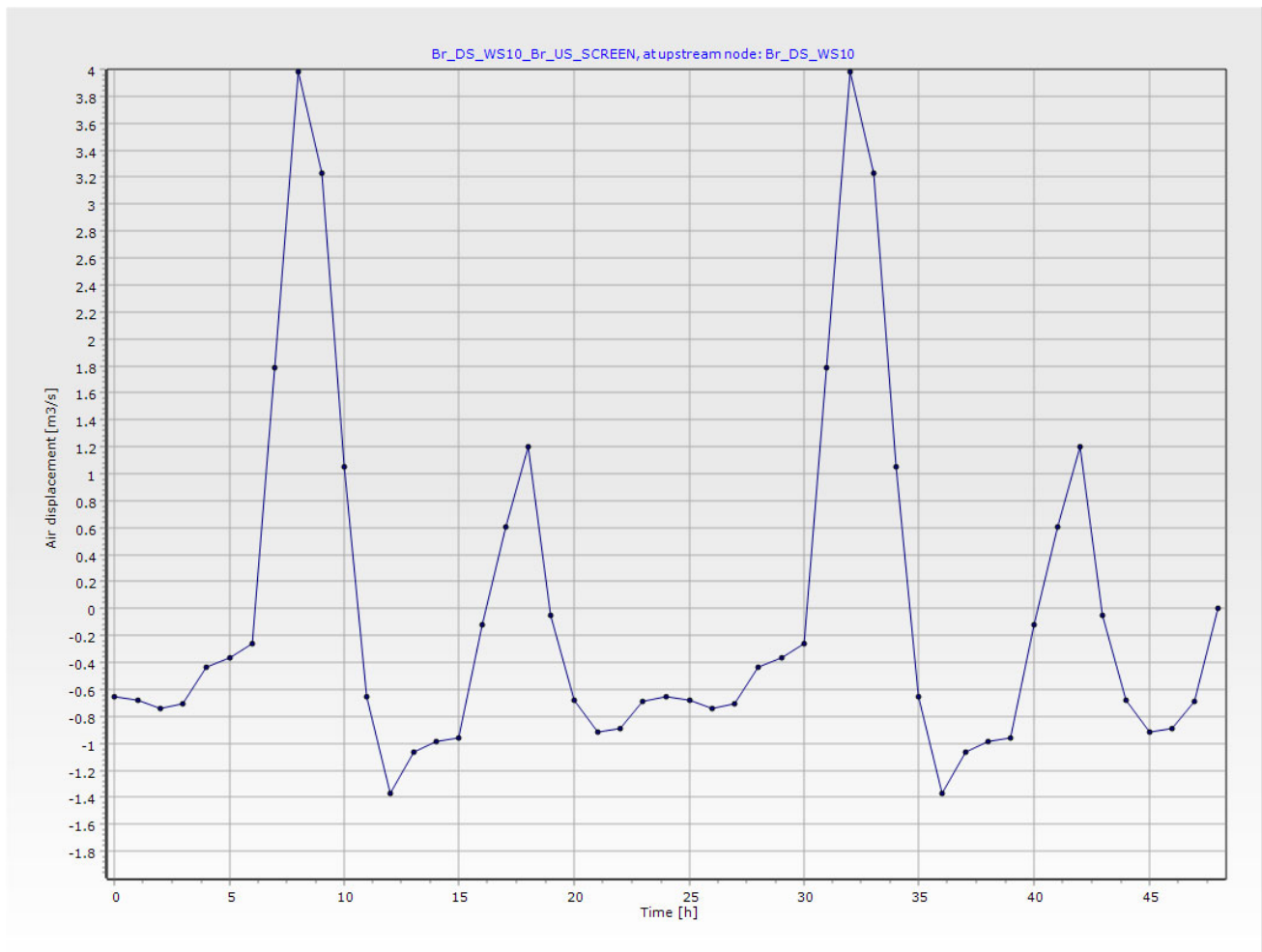


Figure 178. An example of air displacement over the day in a 13 km long tunnel of 4.5 m diameter

## 14 QGIS visualization

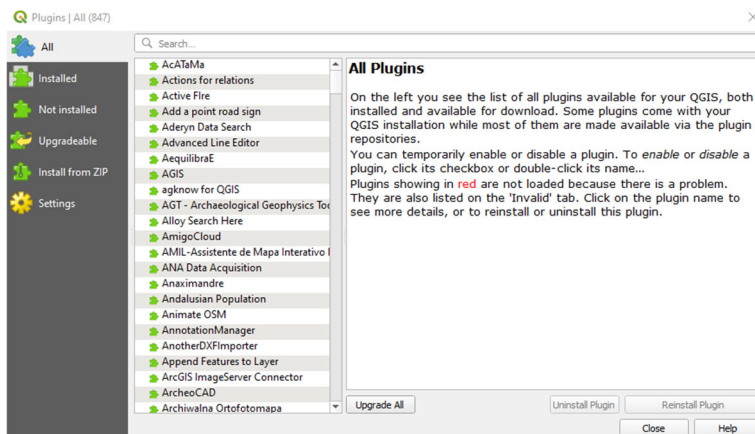
Mega-WATS can export the sewer network and quality data on water and air to a text file format which can be read by QGIS. The format is called Well-Known Text (WKT, [https://en.wikipedia.org/wiki/Well-known\\_text\\_representation\\_of\\_geometry](https://en.wikipedia.org/wiki/Well-known_text_representation_of_geometry)). But before doing this, one needs to install QGIS.

### 14.1 Installing QGIS

QGIS is a free and open-source geographic information system which can be downloaded at [www.qgis.org](http://www.qgis.org). After downloading, one needs to add basemaps to QGIS. Using the QuickMapServices Plugin is probably the easiest way to add basemaps in QGIS. This plugin works with the QGIS 3.0 and later. To add in the plugin, do the following:

- Open QGIS
- Go to Plugins Menu -> Manage and Install Plugins...

The following menu opens



- In the Plugins Window, search for QuickMapServices then click Install button.
- After it installs, you should be able to find QuickMapServices button in the Web Toolbar.



- Click on the button to get the drop-down menu -> Settings.
- In the QuickMapServices Settings window, go to the More Services tab -> Click Get Contributed Pack to get more basemaps.
- Then go to the Visibility tab and turn on/off the basemaps you want to display in the menu (e.g., Bing, Google, etc.)

You should now be able to choose any map and use it as a background layer (note that not all maps in the list work, but if you choose for example Google or Bing, it shall for sure work).

### 14.2 Exporting WKT data from Mega-WATS

Next step is to export data from Mega-WATS into WKT format.

- Go to Output -> QGIS export, and the menu of Figure 178 opens.

**Show data in QGIS format**

Hemisphere  
 Northern hemisphere  
 Southern hemisphere

Transform from a local coordinate system to longitude and latitude: Chose two nodes as far from each other as possible. Get the local coordinates with the "Get upstream (x,y)" buttons. Get the latitude and longitude from a map, Google, Bing, etc., by copy-paste. Push the "Transform (x,y)" button".

	X-coordinate	Y-coordinate	Longitude	Latitude
First node	0.0	0.0	0.00000000	0.00000000
Second node	0.0	0.0	0.00000000	0.00000000

Get upstream (x,y) of pipe 1

Get upstream (x,y) of pipe 2

Get up- or downstream nodes  
 Upstream  Downstream

Central Meridian of zone (degrees) 0  
 Northing offset [m] 0  
 Easting offset [m] 0  
 Roation (degrees) 0  
 Calculated scaling (m/m) 1  
 Radius of Earth at location (m) 6371000

Load coordinate transform settings from separate ini file  Switch between copying longitude/latitude and latitude/longitude

Transform (x,y) coordinates to longitude, latitude      Save coordinate transform settings to separate ini file

---

**Export QGIS network**

Gravity pipes  
 Force mains  
 Special structures  
 All nodes  
 Pump stations  
 Force main discharges  
 Dosing nodes  
 Node callouts  
 x,y callouts  
 Gas equilibrium callouts

Export flow path  
 Export marked pipes

**Export pipe data**

Dissolved sulfide  
 H2S gas  
 Methyl Mercaptan gas  
 Concrete corr. rate  
 Dissolved oxygen  
 Water flow  
 Water velocity  
 Bottom shear stress  
 Air flow  
 Air velocity  
 Air pressure

	Between	and
mg/L	1.0	100000
ppm	1.0	100000
ppm	0.1	100000
mm/y	0.1	100000
mg/L	0.0	10
L/s	0.0	100000
m/s	0.0	100000
Pa	0.0	1
L/s	0.0	10
m/s	0.0	10
Pa	101320	101330

**Export node data**

Air release  
 H2S release  
 MM release  
 Tracer release

	Between	and	Scale
m3/d	0.1	1000000	0.1
g/d	0.001	10000	10
g/d	0.001	10000	10
g/d	0.001	10000	10

Transform a (x,y) coordinate to longitude-latitude

From (x,y)

To (long,lat)

CSV  TAB

CSV  TAB

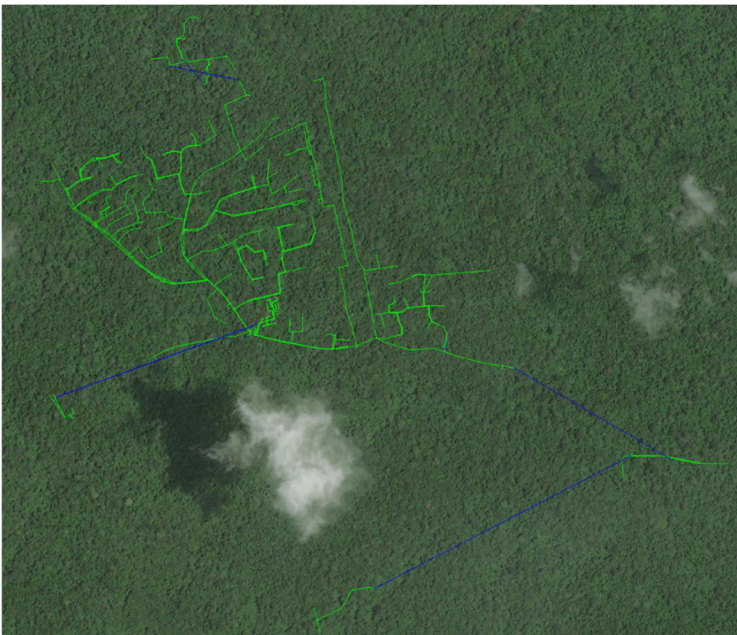
Export pipe data only for pipe flows above  L/s  
 Include force mains  Create high resolution exports

Figure 179. Export to QGIS form (in case pipe ages have not been loaded)

The basemaps of QGIS work with geographic coordinate systems based on longitude and latitude. The Mega-WATS networks are however given in cartesian coordinates (UTM-sort of coordinates), often of local origin. To export to QGIS, the conversion between the two coordinate systems must first be established. The transform parameters needed are

- Northern or Southern hemisphere
- Central meridian of the zone
- Northing offset
- Easting offset
- Rotation
- Scaling




Without these parameters correctly set up, the network will end up somewhere weird, for example like the one below ending up in some forest.



If the network coordinate system is in UTM coordinates, it suffices to write the central meridian of the zone and press export to QGIS buttons.

However, coordinate systems of sewer networks are often in local coordinate systems. To transform these, identify two nodes in the network (preferably as far from each other as possible in north-south and east-west direction). Then find the same nodes on a map (QGIS, or alternatively maps like Google Maps, Bing, OpenStreetMap) and get the longitude, latitude coordinates.

- a. On the Mega-WATS map: Select the pipe which upstream coordinate is to be used
- b. Click button "Get upstream (x,y) of pipe 1". This transfers the Mega-WATS map coordinates to the form as 'First node'.
- c. Go to some map, for example QGIS or Google Maps: Right-click on the map and copy the coordinates to the clipboard. Copy them into the memo-box on the form. Copy the individual coordinates from the memo-box to the Longitude and Latitude cells.
- d. Press the speed-button to the right of the button "Get upstream (x,y) of pipe 1" (marked with a light-blue box in the figure below). This copies the text from the first line of the memo-box into the grid with longitude and latitude. Note that some maps have longitude first and some have latitude first. To swap between which number is copied where, check / uncheck the checkbox marked in yellow (LL).

	X-coordinate	Y-coordinate	Longitude	Latitude	
First node	489673.4	374043.8	0.00000000	0.00000000	Get upstream (x,y) of pipe 1 
Second node	0.0	0.0	0.00000000	0.00000000	Get upstream (x,y) of pipe 2 
-0.6570072, 53.2552527			Load coordinate transform settings from separate ini file 		
Save coordinate transform settings to separate ini file					

- e. Do the same for the second node.
- f. When satisfied, press the button 'Transform (x,y) coordinates to longitude, latitude'. This populates the parameters needed to transform the map.



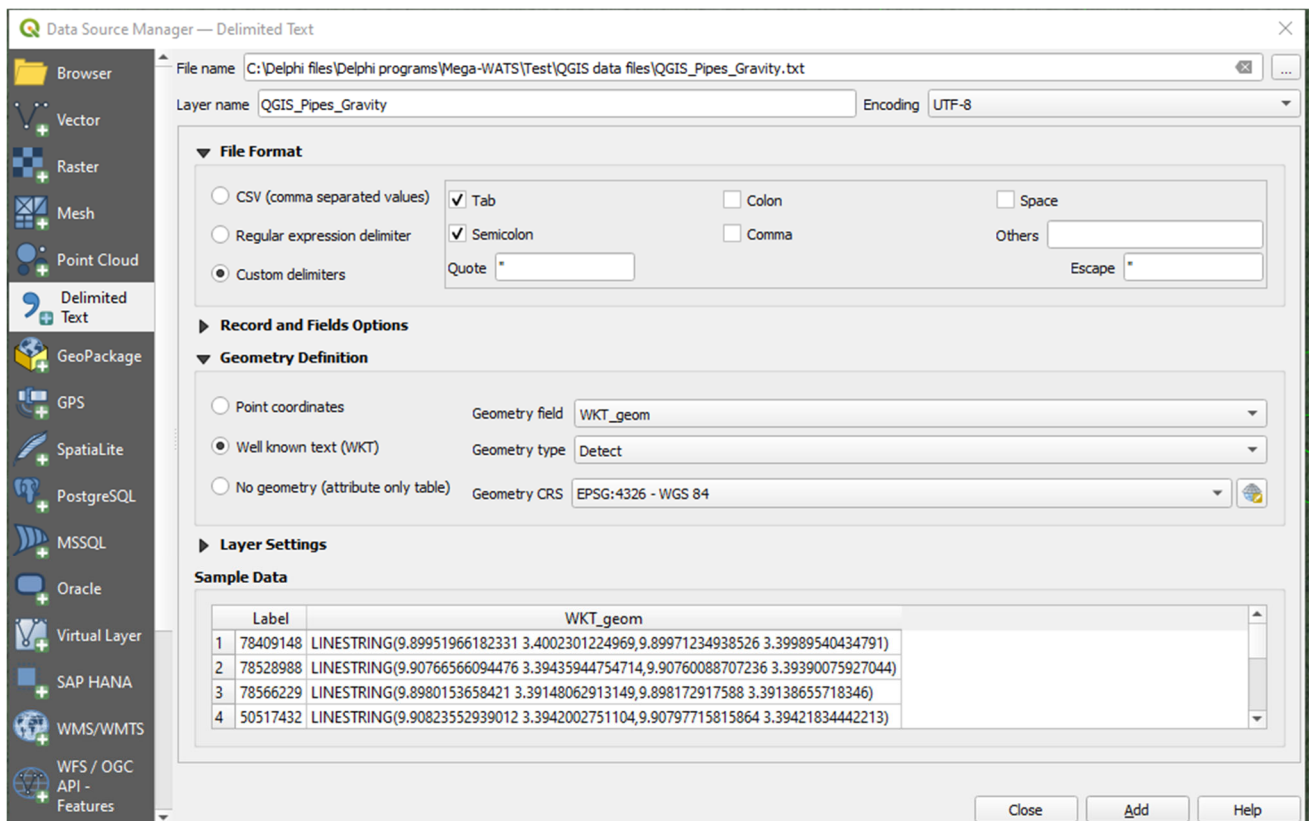
- g. Export the network by pressing “Export QGIS network” and import into QGIS (see below). The first node will now be placed correctly. The second node will likely be a bit off. The reason is that the globe is not a perfect sphere, hence its radius is not the same everywhere. If the network needs to be stretched a bit, then increase the value written under “Radius of Earth at location”. Changes to the radius may be done in steps of 1000 m. Repeat this until the network is placed correctly.

Upon doing this transformation, the data are stored together with general parameters for the simulations. However, it is suggested to also store them in a separate file using the button ‘Save coordinate transformations to separate ini file’, otherwise these data will become lost when resetting the general simulation parameters (the extension of the file is .pam).

After having established the transformation parameters, export information by clicking the export buttons and checking the parameters to be exported. This creates a sub-directory in the folder holding the network file into which the transformation parameters file is placed (...\\QGIS data files\\).

### 14.3 Importing WKT into QGIS

The data files are imported as a delimited text layer. This can be done in QGIS by either choosing Layer -> Add Layer -> Add Delimited Text Layer or by the button ‘Open Data Source Manager’ which leads to the following window opening:



Chose the file in ‘File name’ and import them using the settings shown.

The layers are now visible in QGIS.

## 15 Model calibration

Model calibration is essential to achieving a Mega-WATS model that reflects the real network processes. Effective calibration requires a detailed knowledge of sewer processes as well as experience calibrating numerous projects. Also needed is experience in field observations, sampling, and analysis. For these reasons, it is recommended that every calibration be done jointly between the user and at least one other experienced sewer process modeler. With the experienced sewer process expert and user 'work-shopping' the calibration process, the user will then be made aware of the nuances involved and will thereby build experience needed to become an expert sewer process modeler.



## 16 Working with tracers

Tracers are useful for tracking the fate and transport of a volatile compound across the air water interface and within the sewer network. Any of hundreds of tracers can be represented based on their physical properties. Tracer analysis can, for example, be used to track illicit releases of harmful substances.

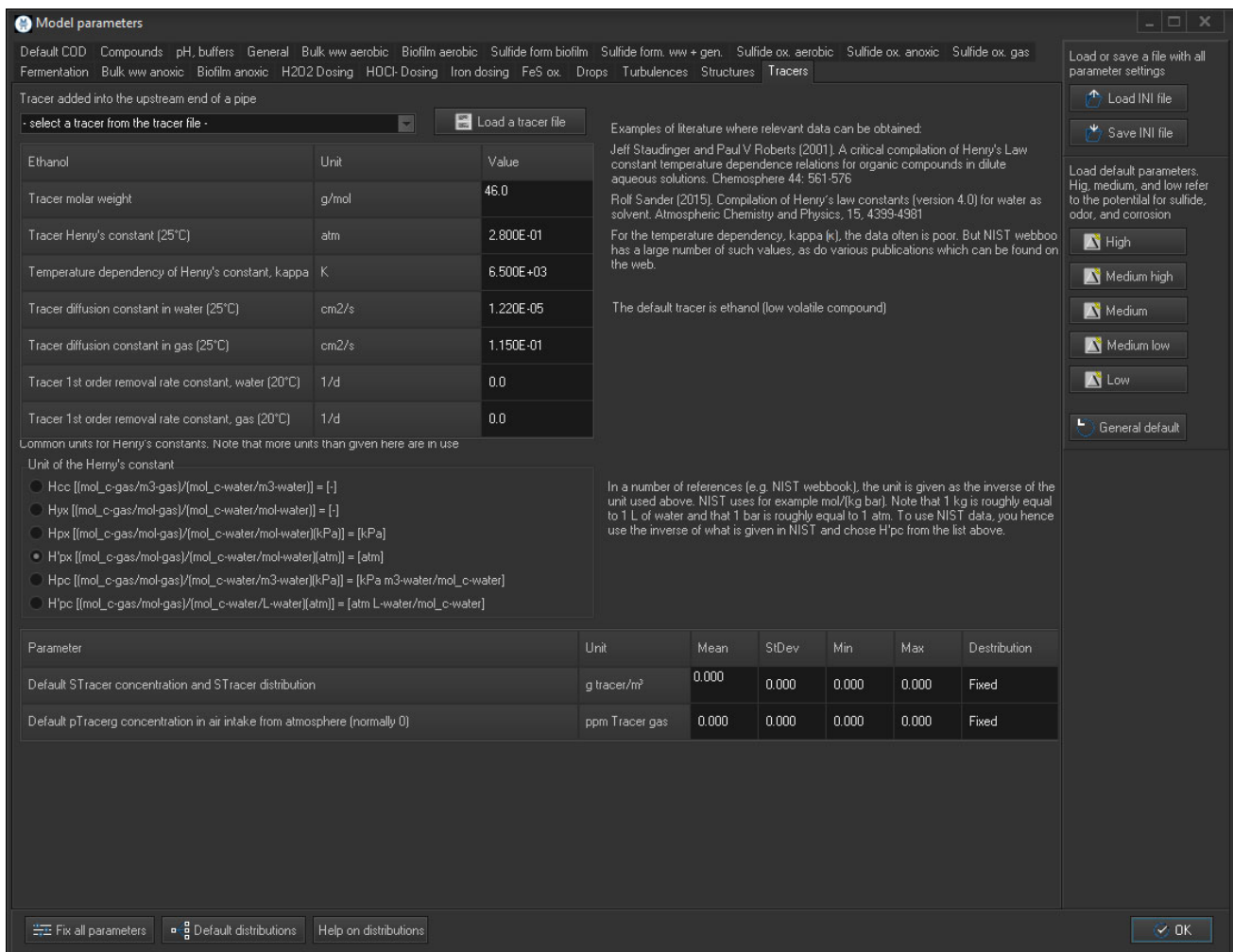
A tracer can be added to the air or to the water as follows:

- A default concentration to all inflows to the network, either in terms of water or air. This is done by stating the default concentrations on the Tracer-page (Figure 179)
- In the matter file for specific inputs to the network (Section 4.2.4)
- As a dosed chemical (Section 4.2.5 and 10.2)

The physicochemical characteristics of a tracer can be chosen freely, and it can be treated as an inert compound or a compound that is slowly removed in the water and the gas.

### 16.1 Setting the physicochemical characteristics of a tracer

The characteristic of a tracer is set in the menu where other model parameters are defined (Figure 179, see also Section 9).



The screenshot shows the 'Model parameters' window with the 'Tracers' tab selected. The 'Tracer added into the upstream end of a pipe' dropdown is set to 'select a tracer from the tracer file'. The 'Load a tracer file' button is visible. The main table lists the following parameters for Ethanol:

Parameter	Unit	Value
Tracer molar weight	g/mol	46.0
Tracer Henry's constant (25°C)	atm	2.800E-01
Temperature dependency of Henry's constant, kappa	K	6.500E+03
Tracer diffusion constant in water (25°C)	cm <sup>2</sup> /s	1.220E-05
Tracer diffusion constant in gas (25°C)	cm <sup>2</sup> /s	1.150E-01
Tracer 1st order removal rate constant, water (20°C)	1/d	0.0
Tracer 1st order removal rate constant, gas (20°C)	1/d	0.0

Below the table, there are sections for 'Common units for Henry's constants' and 'Unit of the Henry's constant' with several radio button options. A 'Distribution' table is also present at the bottom of the window:

Parameter	Unit	Mean	StDev	Min	Max	Distribution
Default STracer concentration and STracer distribution	g tracer/m <sup>3</sup>	0.000	0.000	0.000	0.000	Fixed
Default pTracerg concentration in air intake from atmosphere (normally 0)	ppm Tracer gas	0.000	0.000	0.000	0.000	Fixed

On the right side of the window, there are buttons for 'Load or save a file with all parameter settings' (Load INI file, Save INI file) and 'Load default parameters' (High, Medium high, Medium, Medium low, Low, General default). At the bottom right, there is an 'OK' button.

Figure 180. Setting up tracers and their physicochemical characteristics

Tracers can be manually defined by typing their physicochemical characteristics in the string grid. The data needed for a tracer are:

- The molecular weight of the tracer in the unit of g/mol
- The Henry’s constant of the tracer at 25°C. In the literature, the Henry’s constant comes in a wide range of units which can be quite complex to transfer to what one needs. There are hence given six of the most common units of the Henry’s constant, and Mega-WATS will transform between them when clicking the radio buttons of the constants. Henry’s constant can be found in specialized literature, for example Staudinger and Roberts (2001) or in Sander (2015). Note that in several references (e.g., NIST webbook), the unit is given as the inverse of the unit used above. NIST uses for example mol/(kg bar). Note that 1 kg is roughly equal to 1 L of water and that 1 bar is roughly equal to 1 atm. To use NIST data, you hence use the inverse of what is given in NIST and chose H'pc from the list of Henry’s constants units.
- The temperature dependency of the Henry’s constant. It is well known that mass transfer equilibria are temperature dependent, for example, oxygen is more soluble in cold water than in warm water. For the temperature dependency, kappa ( $\kappa$ ), the data often is poor. But NIST webbook has many such values, as do various publications which can be found on the web.
- Diffusivity in water and gas. The diffusion constant for the tracer in the water and the gas are needed in the calculation of how a substance is transferred between water and gas. WATS applies the two-film theory for calculating mass transfer as described in Matias et al. (2018).
- Removal rate constants. The tracer can be treated as inert or as undergoing a removal process. If the rate constants are set to zero, the tracer is inert. A value in the air or gas or both will lead to a removal following a simple first order removal process in the tracer concentration ( $dC/dt = -kC$ ).

## 16.2 Adding tracers from a file

In the upper left corner is a drop-down menu showing pre-defined tracers. These are stored in a file which the user can edit like other Mega-WATS input files and the file must be loaded before using these.

The format of the file is shown in Table 11. The first two rows of the file are only information for the user and can contain anything.

Table 11. The format of the tracer file

	Henry's constant	Henry's unit	Henry's kappa	Molar weight	Diffusivity in water	Diffusivity in air	1st order removal rate constant, water	1st order removal rate constant, water
	[atm]		[K]	[cm <sup>3</sup> mol <sup>-1</sup> ]	[cm <sup>2</sup> s <sup>-1</sup> ]	[cm <sup>2</sup> s <sup>-1</sup> ]	[d <sup>-1</sup> ]	[d <sup>-1</sup> ]
Ethanol	0.28	3	6500	46.0	1.22E-05	0.115	0.000	0.000
Acetone	2.06	3	4800	74.0	1.20E-05	0.109	0.000	0.000
Methyl mercaptan	166	3	2800	55.2	1.43E-05	0.130	0.000	0.000
Oxygen	4.20E+04	3	1700	25.6	2.24E-05	0.235	0.000	0.000

The column ‘Henry’s unit’ indicates the unit in which the constant is given:

- 0  $H_{cc} [(mol\_c-gas/m^3-gas)/(mol\_c-water/m^3-water)] = [-]$
- 1  $H_{yx} [(mol\_c-gas/mol-gas)/(mol\_c-water/mol-water)] = [-]$
- 2  $H_{px} [(mol\_c-gas/mol-gas)/(mol\_c-water/mol-water)(kPa)] = [kPa]$
- 3  $H''_{px} [(mol\_c-gas/mol-gas)/(mol\_c-water/mol-water)(atm)] = [atm]$
- 4  $H_{pc} [(mol\_c-gas/mol-gas)/(mol\_c-water/m^3-water)(kPa)] = [kPa\ m^3-water/mol\_c-water]$
- 5  $H''_{pc} [(mol\_c-gas/mol-gas)/(mol\_c-water/L-water)(atm)] = [atm\ L-water/mol\_c-water]$

### 16.3 Adding a tracer as a chemical

A tracer is added in the same way as other chemicals (Section 4.2.5 and 10.2). It can be added via the *Chemical dosing* file, where a tracer added to the water is termed *TracerW*, while one added to the gas is termed *TracerG*. The file contains the following fields (see the example spreadsheet for information on how to set up this file):

- The identifier of the pipe at which upstream end the tracer is added
- The unit for adding the tracer. Either  $g/m^3$  or  $g/s$ . If  $g/m^3$  is chosen for the water phase, the responding water phase concentration becomes this concentration. The same is the case for the gas phase addition, however, the unit of  $g/m^3$  of tracer in the air is subsequently transformed by Mega-WATS to ppm on a mole fraction basis, i.e., corresponding to the partial pressure of the tracer in the gas. If  $g/s$  is chosen, the tracer flow is mixed into the water stream or gas stream. For the water stream it is assumed that the tracer concentration is 500  $g/L$ , hence adding 2  $L/s$  of water for each  $kg/s$  of tracer. For the gas it is assumed that the tracer is a pure gas, meaning that for each  $L$  of tracer gas at atmospheric pressure, the air flow is increased by 1  $L/s$ .
- The average addition of the tracer
- The diurnal variation of the tracer

A tracer can also be added at runtime applying the 'Dose to' button in the lower left part of the user interface. When opening the dialog, the two tracer options are shown to the right (Figure 180).

- Choose one of the tracer options and one of the dose units' options.
- Write a concentration to dose.
- Press the 'Dose' button.

One can now close the form and run the model

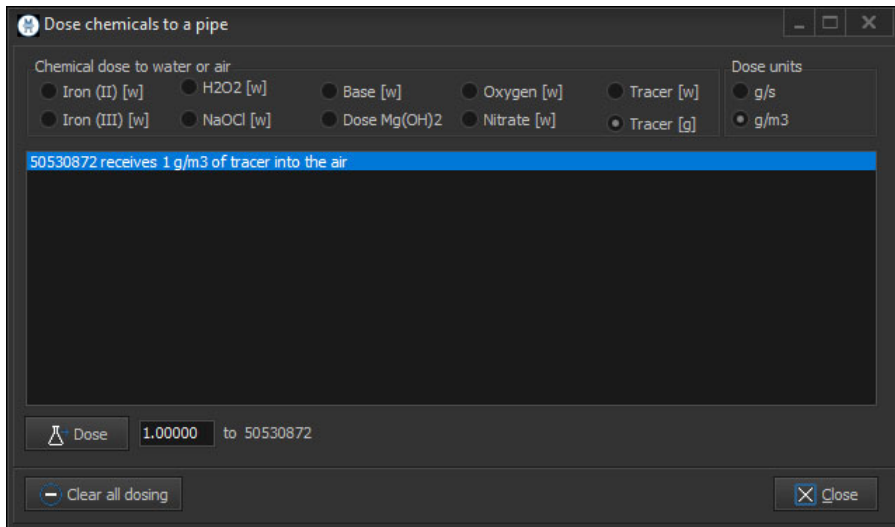


Figure 181. The dosing menu used for adding a tracer

Mega-WATS will store this information for the next time the model is run. If one wants to remove the dosing, one can either open the *Build a project* form (section 4.1) and clear the dosing by pressing the *Clear all dosing* button, or one can re-open the dose dialog window and dose zero to the same pipe. When doing so, make sure this pipe is selected. One can select the pipe on the map, by clicking the pipe name in the dialog below the *Dose to* button (Figure 180), or in the pipe list-box at the top left corner of the user interface (Figure 181). Make also sure you press the tracer (or chemicals) type you want to remove. Write zero in the input line. Then press the *Dose to* button and the line (and dosing) disappears.

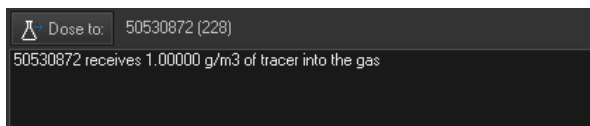


Figure 182. The list-box showing which pipes receive a tracer (or dosing of any other chemical)

#### 16.4 Running a simulation with a tracer

The behavior of your tracer addition will depend strongly on its physicochemical characteristics. To exemplify this, a simulation of a part of a network is shown in Figure 182. The flow in the pipes of the path is shown in Figure 183.

In the first example the tracer is insoluble in air, inert, and added to the water phase (Figure 184). An example could be a salt, like sodium chloride. To achieve this, the Henry's constant is set to zero (Figure 179).

In the second example the tracer has a medium solubility in the air, inert, and added to the water phase. The resulting water and air phase concentrations are shown in Figure 185 and Figure 186, respectively.

In the second example the tracer has a high solubility in the air, inert, and added to the water phase. The resulting water and air phase concentrations are shown in Figure 187 and Figure 188, respectively.

A tracer can also be added to the air of the sewer (Figure 189 and Figure 190). This would typically be a tracer of low solubility in water (high solubility in air). If the tracer is insoluble in water, the Henry's constant is set to zero or to a very high value.

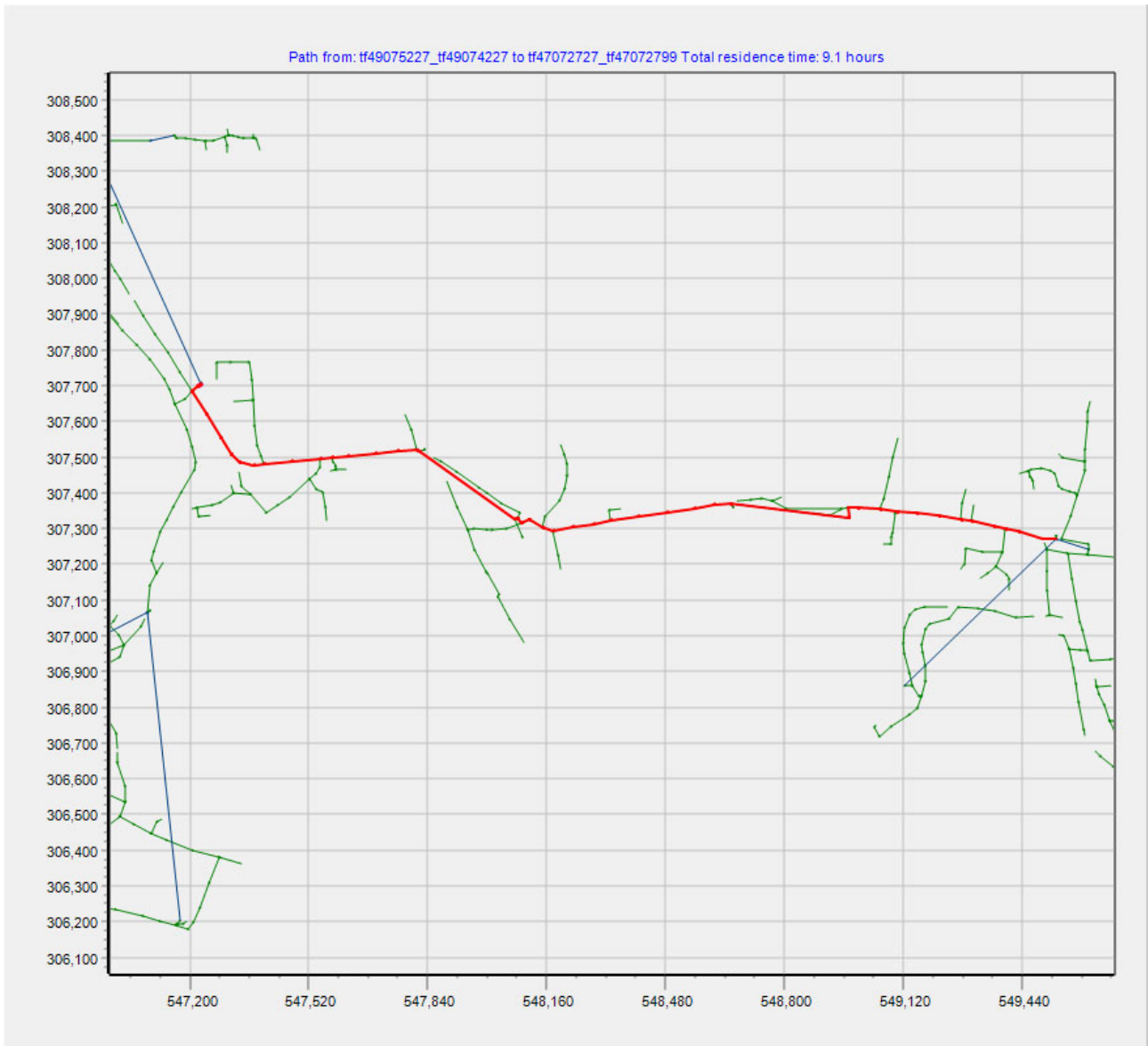


Figure 183. Flow path for tracer example

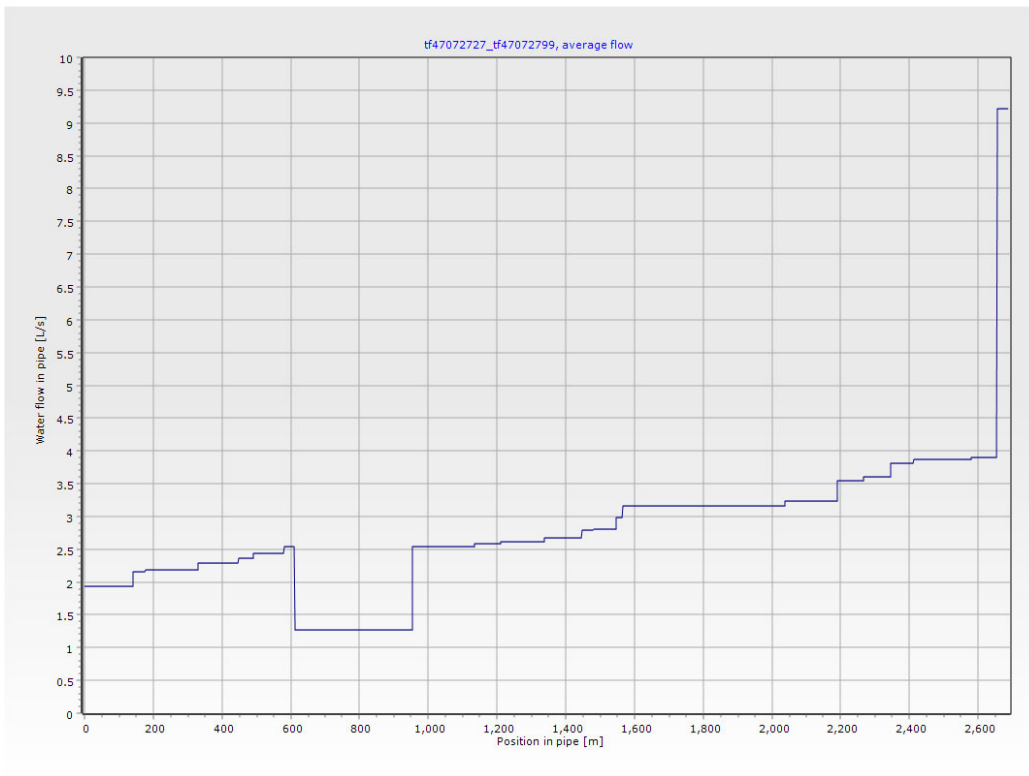


Figure 184. Flow in the path shown in Figure 182. The drop in flow at position 600-950 is due to two force mains running in parallel

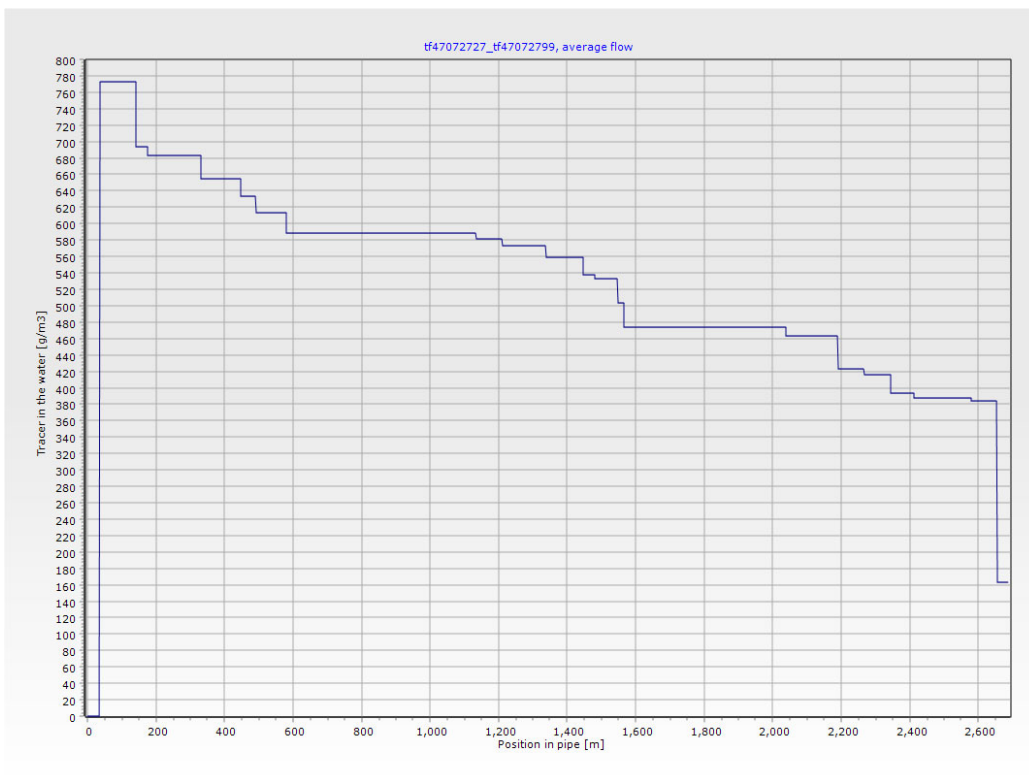


Figure 185. Tracer in the water along the flow path of Figure 182. An inert tracer which cannot be transferred to the air (insoluble in air) is added to the water.

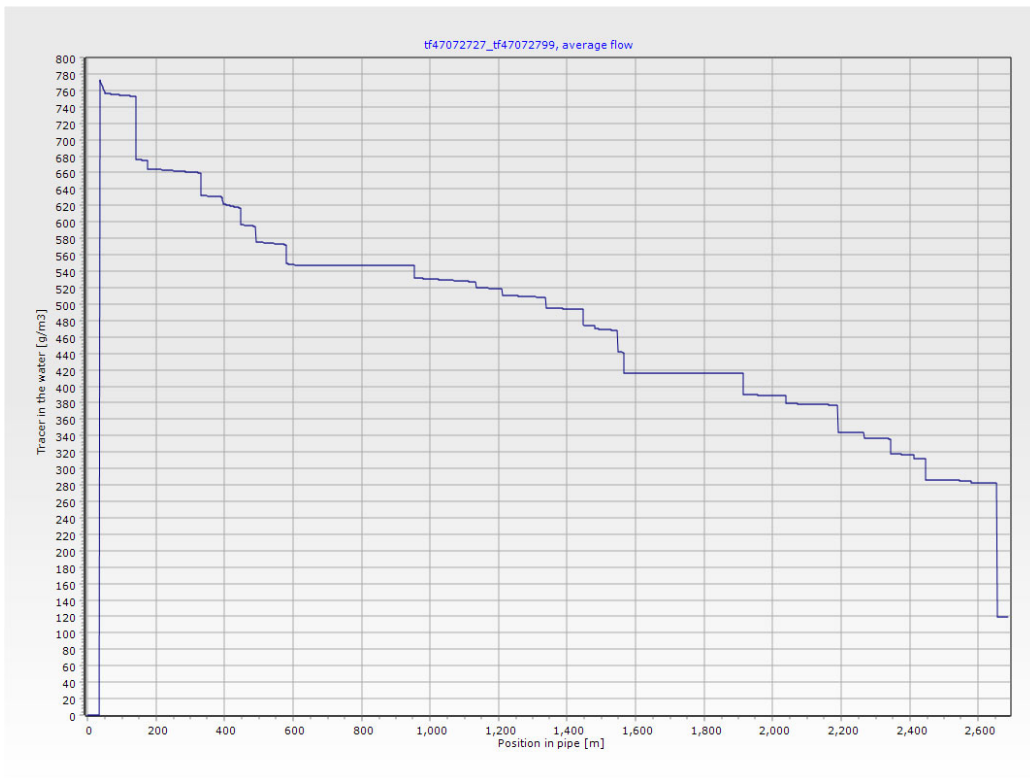


Figure 186. Tracer in the water along the flow path of Figure 182. A tracer with a medium solubility in air is added to the water.

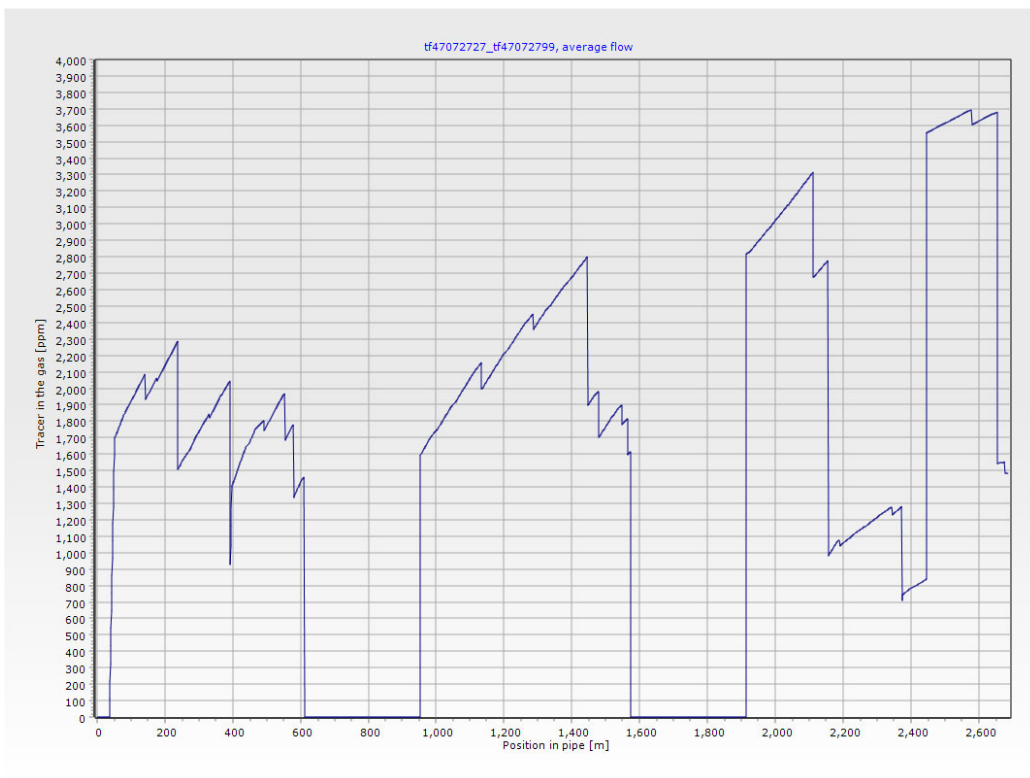


Figure 187. Tracer in the gas along the flow path of Figure 182. A tracer with a medium solubility in air is added to the water.



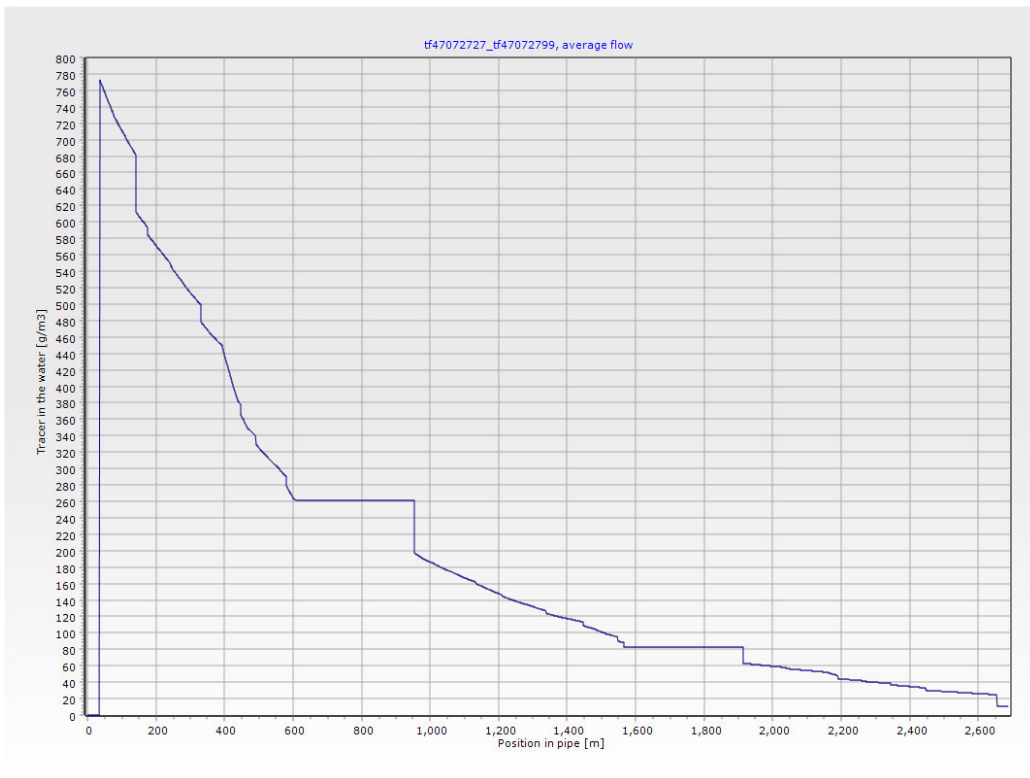


Figure 188. Tracer in the water along the flow path of Figure 182. A tracer with a high solubility in air is added to the water.

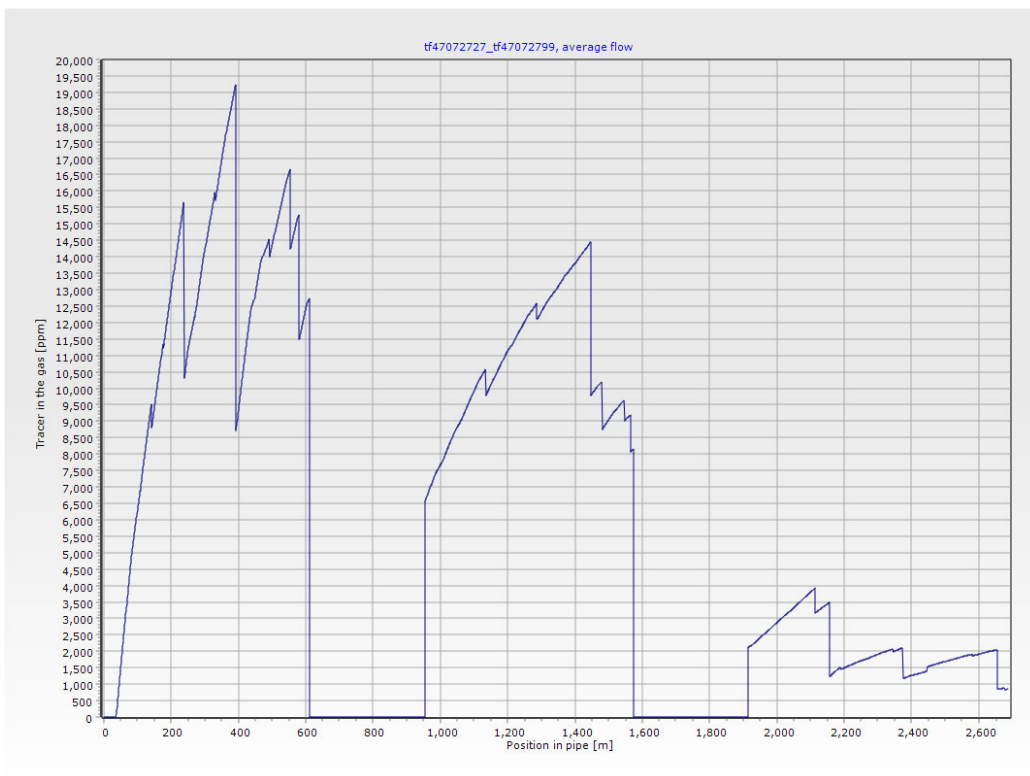


Figure 189. Tracer in the air along the flow path of Figure 182. A tracer with a high solubility in air is added to the water.

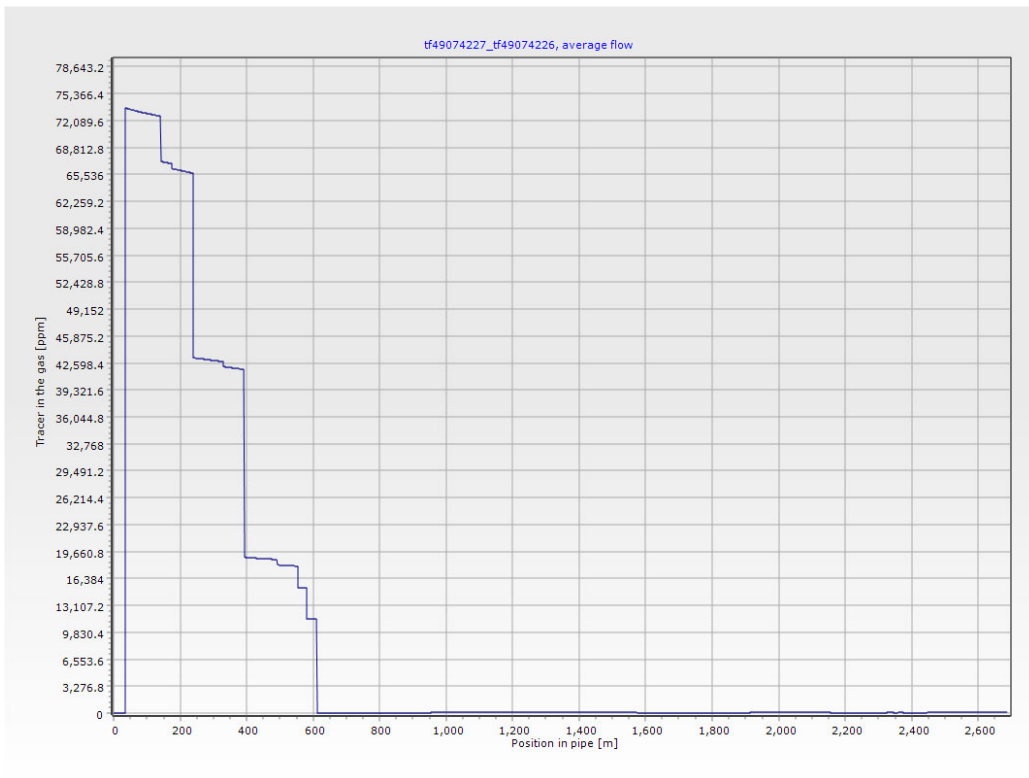


Figure 190. Tracer in the air along the flow path of Figure 182. A tracer with a high solubility in air is added to the air. The reason the concentration drops drastically at 600 m is that the flow here enters a force main

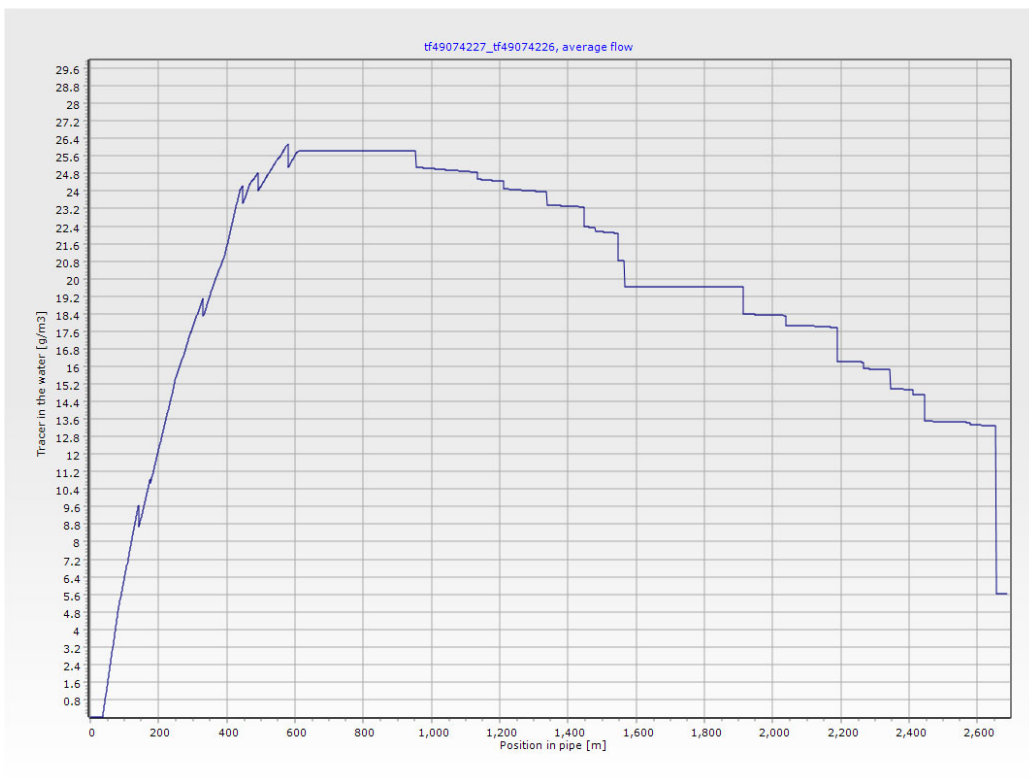


Figure 191. Tracer in the water along the flow path of Figure 182. A tracer with a high solubility in air is added to the air.

### 16.4.1 Special considerations for gases with low Henry's constant

Gases with low Henry's constant must be modelled at a smaller space step than other gases as results otherwise are numerically unstable. One example is ammonia, which must be simulated at space steps as low as 0.01 – 0.1 m instead of the 1 m which is the default setting of Mega-WATS.

### 16.5 Off-gas from the network

Tracer off-gassing can be shown as described in general for off-gas in section 6.3.16, and an integrated value of off-gas within some distance of a point can be calculated (Figure 191).

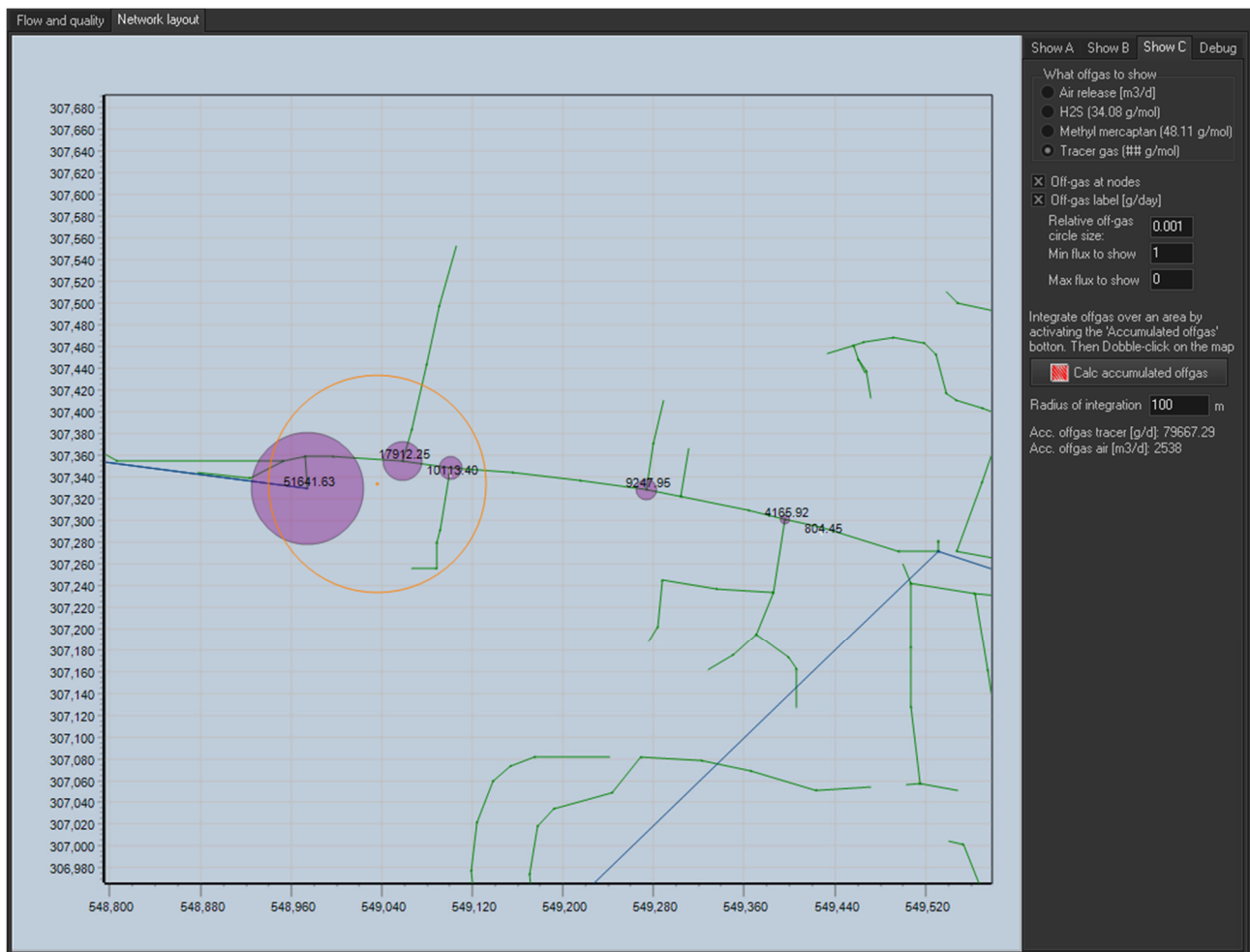


Figure 192. Tracer off-gas where a tracer with a high solubility in air is added to the air.

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