Tutorial

ELV-EQS web-based software

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Contents

1 Introduction

The ELV-EQS web-based tool was developed to establish a relationship between environmental quality standards (EQSs) in receiving water bodies and emission limit values (ELVs) for a single pollutant discharge. Based on the user-defined characteristics of the discharge, the pollutant, and the receiving water body, the tool calculates the dispersion of the pollutant within the water body and compares its ELVs with the EQSs at the edge of the allowable mixing zone.

This Tutorial Document can be used to get acquainted with the procedure to set up a site-specific application of the ELV-EQS tool. It guides the user through the set-up of a scenario using all the functionalities of the ELV-EQS tool.

Two tutorials (hereafter also referred to as "cases") have been selected based on the findings of the project "*Testing of a modelling system to assess the variations of EQSs with ELVs for nitrogen and mercury in Gulf of Lion and Izmir Bay*" (Deltares 2012), and are described in the following.

The first test-case (Tutorial 1) investigates the effects of a discharge of total nitrogen within an open environment such as the coastal area in front of Marseille (Gulf of Lion). The second test-case (Tutorial 2) deals with the impact of a discharge of total mercury within an enclosed bay, such as the Izmir Bay (Aegean Sea).

2 Clauses

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3 Tutorial 1: Discharge of total nitrogen in the Gulf of Lion

The ELV-EQS tool can be accessed via the internet at [*TODO: specify URL]*.

3.1 Setup of the case

The setup of a "case" in the ELV-EQS tool is done in three stages. The first step is to describe the environment where the discharge will occur (Environment description). The second step is to provide information on the discharge itself (Discharge description). Finally, the last step in setting up your "case" is to describe the substance that is discharged and its allowable limits within the area of interest (Substance properties).

3.1.1 Environment description

The first example focuses on the Eastern part of the Gulf of Lion, along the coast near Marseille (Figure 3.1). The area of interest is best described as an "open" environment[1]. The dimensions of the area are fixed to 5,000 m (length) x 2,000 m (width). To account for the orientation of the coastline in this part of the Gulf, the computational grid is rotated by 145 degrees clockwise[2].

[1] An "open" computational grid consists of 1 closed boundary and 3 open boundaries. An "enclosed" computational grid consists of 1 open boundary and 3 closed boundaries.

[2] See (GUID) for a description on how to calculate the rotation of the grid.

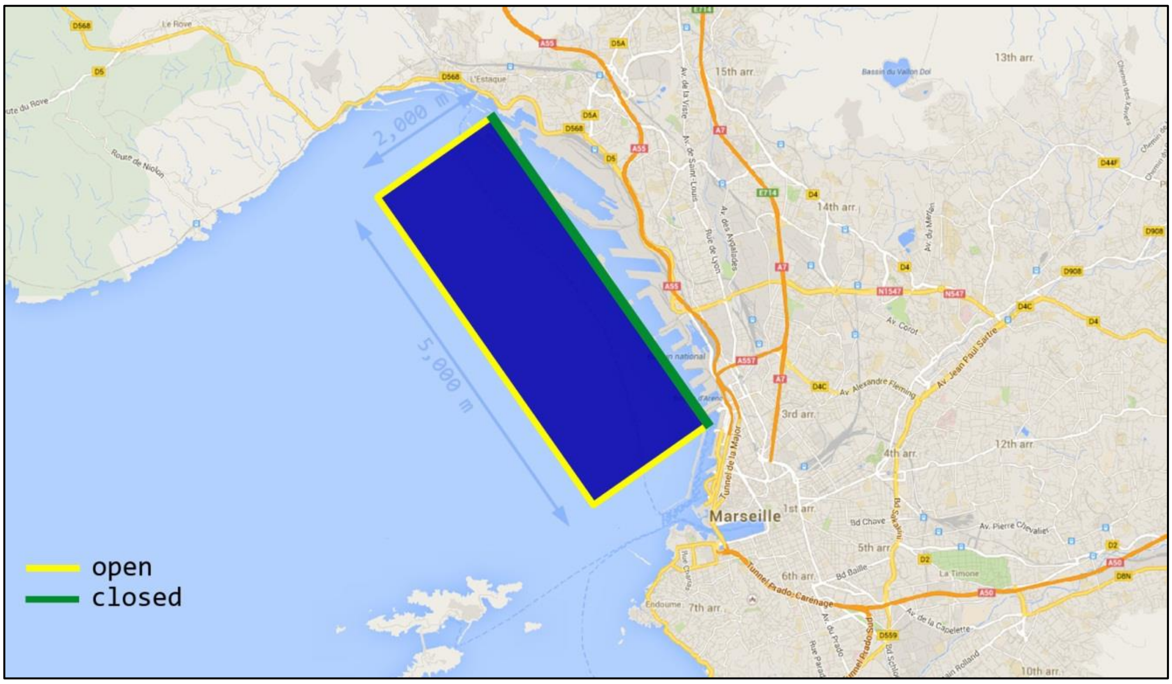


Figure 3.1 Schematization of the "open" computational grid in Marseille Bay (Eastern part of the Gulf of Lion).

Based on the available bathymetric data (Berné et al. 2004, Deltares 2012), the water depth from near-shore to the offshore boundary increases from 20 to 60 m, resulting in a bottom slope of 0.02 m/m (i.e. 40 m depth over a horizontal distance of 2,000 m).

The ELV-EQS tool allows for an assessment including up to 10 meteorological/current alternatives. In this first example, however, only one meteorological/current alternative is used.

The dominant wind conditions experienced in the Gulf are chosen based on the available meteorological information (see Deltares 2012), and are assumed to occur during 100% of the time. Therefore, the predominant wind direction is North-Westerly (320 degrees), with an average speed of 5.8 m/s at 10 m above the ground.

Velocity measurements in the centre of the study area revealed a stagnant character for the water in Marseille Bay (Vousdoukas et al. 2011), with maximum flow velocities of 0.1 m/s near the bed. For the present example, we will use a current velocity of 0.05 m/s.

The ambient water temperature ranges from 13 to 25 degrees C, and the ambient salinity reaches 38 ppt in the bay (Pairaud et al. 2011). In this example, the background water temperature is therefore fixed at 20 degrees C and the ambient salinity at 38 ppt (above pycnocline). Furthermore, information regarding the concentration of suspended solids is lacking. Therefore, we use a value of 20 mg/L, as discussed in Deltares (2012).

All the values relevant to the environment description are summarized in Table 3.1.

Table 3.1 Properties of the environment

Name	Value
Study area	
Type of environment	Open
Size of simulation domain L1 along the coast	5,000 m
Size of simulation domain L2 perpendicular to the coast	2,000 m
Orientation of study area relative to North	145 degrees
Water depth near-shore	20 m
Bottom slope	0.02 m/m
Meteo/current alternatives	
Number of different meteo/current alternatives	1
Frequency of occurrence	100%
Wind speed at 10 m above water surface	5.8 m/s
Wind direction relative to North	320 degrees
Current speed	0.05 m/s
Receiving water characteristics	
Suspended solids concentration	20 g/m^3
Salinity (above pycnocline)	38 ppt
Temperature (above pycnocline)	20 degrees C

After starting the tool, the user can enter these values in the relevant fields, as shown in Figure 3.2.

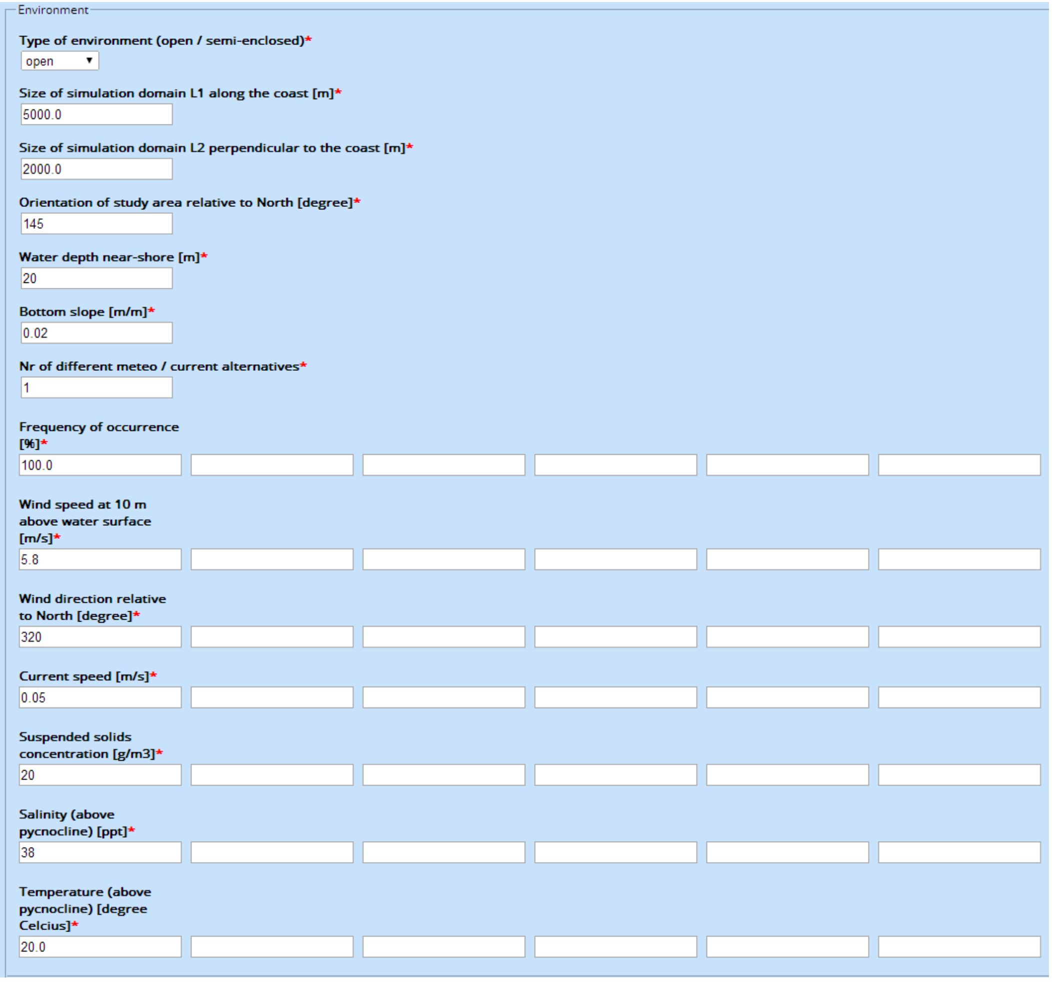


Figure 3.2 Definition of the receiving water characteristics in the ELV-EQS tool for Case 1.

3.1.2 Discharge description

The location of the discharge is chosen along the coastline-side, very close to Marseille. It is located in the longitudinal middle of the grid (X1=2,500 m), and 100 m away for the border of the domain (X2=100 m). Additionally, the discharge is located at the surface of the water column (depth=0 m).

In the following, we consider a fresh water discharge containing the simulated pollutant (total nitrogen). Salinity of the discharge is equal to 0.0 ppt, while the water temperature is fixed at 20 degrees C. Furthermore, it is assumed that the water discharged does not contain particles. Assuming a flow rate of 15 m^3/h (i.e. 0.25 m^3/s) and a load of 1 g/s of the simulated pollutant, the concentration of the simulated pollutant is then 4 g/m^3. Besides, we assume that the discharge occurs from a pipe with a diameter of 0.2 m.

All the values relevant to the discharge characteristics are summarized in Table 3.2.

Table 3.2 Properties of the discharge

Name	**Value**
Position of discharge along the coast (X1)	2,500 m
Position of discharge from the coast (X2)	100 m
Position of discharge from water surface (depth)	0.0 m
Discharge rate	15 m^3/h
Discharge pipe opening diameter	0.2 m
Discharge temperature	20 degrees C
Discharge salinity	0.0 ppt
Discharge concentration chemical of concern	4 g/m^3
Discharge concentration of suspended solids	0.0 g/m^3

The user can now enter these values in the relevant fields of the ELV-EQS tool, as shown on Figure 3.3.

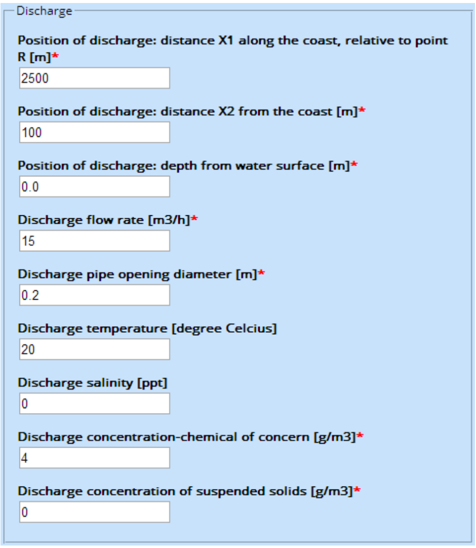


Figure 3.3 Definition of the discharge characteristics in the ELV-EQS tool for Case 1.

3.1.3 Substance properties

In this example, we focus on the discharge of total nitrogen. For nitrogen, we consider denitrification as a process which effectively removes nitrogen from the aquatic environment (Herbert 1999). Based on available information (EPA 1985, Deltares 2012), a decay rate of 0.03 d^{-1} is selected for the present case.

In the case of nitrogen, we do not use a partition coefficient (= 0.0 m^3/kg) since EQS values are commonly expressed as "total concentration of nitrogen" and refer to the sum of the particulate and the dissolved fractions.

For sake of simplicity, a nil background concentration of total nitrogen (0.0 g/m^3) is assumed.

In addition, the Water Framework Directive (2000/60/EC) does not formulate EQSs for nitrogen at a European level. In the following, we therefore assume an EQS for maximum allowable concentration equal to 10 g/m^3 and an EQS for annually averaged concentration equal to 0.4 g/m^3 (based on expert judgement). The sizes of the mixing zones for the maximum allowable concentration and for the annually averaged concentration are assumed to be identical and equal to 500 m.

Because the ELV-EQS tool is a so-called “rapid assessment tool”, it should adopt a worst-case approach: the simplifications of the tool should never lead to the acceptance of a discharge that would have been rejected in a more detailed assessment. For that reason, we use a safety factor for fate and transport calculation (Deltares 2012). Its value is fixed to 2.

Values describing the properties of the substance discharged are summarized in Table 3.3.

Table 3.3 Properties of the substance

Name	**Value**
Name of the Substance	Total nitrogen
Substance Decay rate	0.03 d^{-1}
Substance Partition Coefficient	0.0 m^3/kg
Background concentration	0.0 g/m^3
EQS (MAC, maximum allowable concentration)	10 g/m^3
Allowable mixing zone (MAC)	500 m
EQS (AA, annually averaged concentration)	0.4 g/m^3
Allowable mixing zone (AA)	500 m
Safety factor for fate and transport calculation	2

The user can now enter these values in the relevant fields of the ELV-EQS tool, as shown in Figure 3.4.

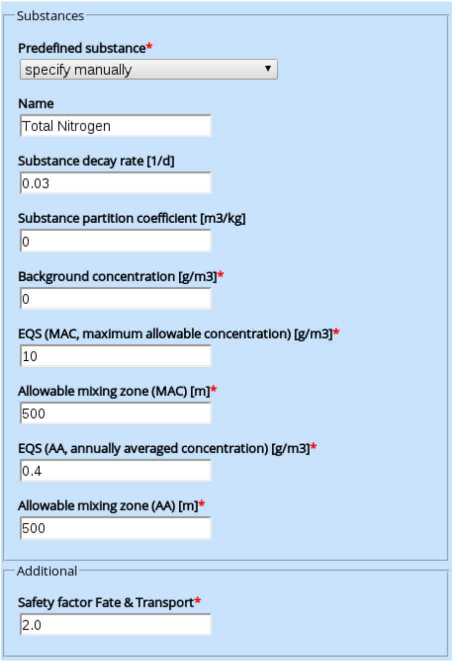


Figure 3.4 Definition of the substance properties in the ELV-EQS tool for Case 1.

Note that it is also possible to select this substance from the list of predefined substances in the dropdown menu. In that case the name, decay rate and partition coefficient do not have to be entered manually.

3.2 Computation

At this point, if you wish to save your input data, use the "Save" button to store all the input information into a text file. Later, you can simply load the text file into the ELV-EQS tool by first selecting the file (using the "Browse" button) and then loading it into the webpage (using the "Load" button), as illustrated in Figure 3.5.

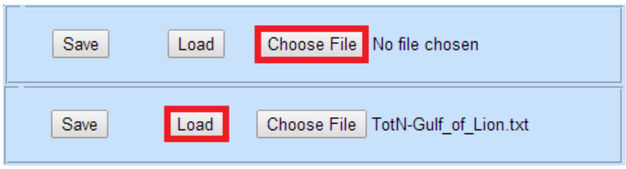


Figure 3.5 Importing input from a saved scenario. Select "Choose File" to browse for the file. Once chosen, the file name appears next to the button. Select "Load" to load the input data into the ELV-EQS tool.

When all the (correct) information is supplied to the ELV-EQS tool, the "case" can be submitted to the computational core, which will then display the results after a quick computation.

For that purpose, click the button "Submit" at the bottom of the webpage, as shown in Figure 3.6.

Figure 3.6 Submit your case to the computational core to obtain the results.

3.3 Results

After the case has been submitted and the calculations have been performed, the webpage displays a page containing the results of the simulation (Figure 3.7). These are presented in a tabular format, showing the annual mean and maximum concentrations of the chemical of concern (here total nitrogen) at an increasing distance from the source (from 0 to 2,000 m).

Distance from pipe [m]	Maximum concentration [g/m3]	Mean concentration [g/m3]
0.	8.000000E+00	8.000000E+00
10.	5.040323E-01	5.040323E-01
20.	3.140580E-01	3.140580E-01
30.	2.593109E-01	2.593109E-01
40.	2.148747E-01	2.148747E-01
50.	1.908351E-01	1.908351E-01
60.	1.695346E-01	1.695346E-01
70.	1.546641E-01	1.546641E-01
80.	1.417384E-01	1.417384E-01
90.	1.329522E-01	1.329522E-01
100.	2.630253E-03	2.630253E-03
200.	1.841183E-03	1.841183E-03
300.	1.347679E-03	1.347679E-03
400.	1.028226E-03	1.028226E-03
500.	8.139774E-04	8.139774E-04
600.	6.651040E-04	6.651040E-04
700.	5.580405E-04	5.580405E-04
800.	4.785105E-04	4.785105E-04
900.	4.189385E-04	4.189385E-04
1000.	3.832673E-04	3.832673E-04
1200.	3.251345E-04	3.251345E-04
1400.	2.803598E-04	2.803598E-04
1600.	2.450458E-04	2.450458E-04
1800.	2.165140E-04	2.165140E-04
2000.	1.938384E-04	1.938384E-04

Figure 3.7 Results page showing the calculated maximum and averaged concentration at several distances from the source of the discharge.

In addition, the EQS, the size of the mixing zone, the concentration at the edge of the mixing zone, and a compliance check are summarized in a table for the maximum concentration and the annual mean concentration of the chemical of concern (Figure 3.8). This allows the user to quickly assess whether or not the discharge is permitted, and if not, where the threshold is exceeded.

description	Maximum concentration [g/m3]	Mean concentration [g/m3]
EQS	1.000000E+01	4.000000E-01
defined mixing zone	5.000000E+02	5.000000E+02
concentration at edge of defined mixing zone	8.139774E-04	8.139774E-04
discharge permitted?	YES	YES

Figure 3.8 Summary table indicating the results of the compliance check.

In this first example, the compliance with the EQS for maximum (10 mg/L) and annual mean concentration (0.4 mg/L) of total nitrogen is met at the edge of their respective mixing zones (500 m for both). Maximum and annual mean concentrations are equal in this case, since the scenario only consists of one wind/current alternative. The discharge is therefore permitted.

4 Tutorial 2: Discharge of total mercury in Izmir Bay

The ELV-EQS tool can be accessed via the internet at *[TODO: specify URL]*.

4.1 Setup of the case

The setup of a "case" in the ELV-EQS tool is done in three stages. The first step is to describe the environment where the discharge will occur (Environment description). The second step is to provide information on the discharge itself (Discharge description). Finally, the last step in setting up your "case" is to describe the substance that is discharged and its allowable limits within the area of interest (Substance properties).

4.1.1 Environment description

The second example focuses on Izmir Bay, located in the Eastern part of the Aegean Sea (Figure 4.1). The area of interest is best described as an "enclosed" environment[3]. The dimensions of the area are fixed to 2,000 m (length) x 5,000 m (width). To account for the orientation of the coastline in this part of the Aegean Sea, the computational grid is rotated by 150 degrees clockwise[4].

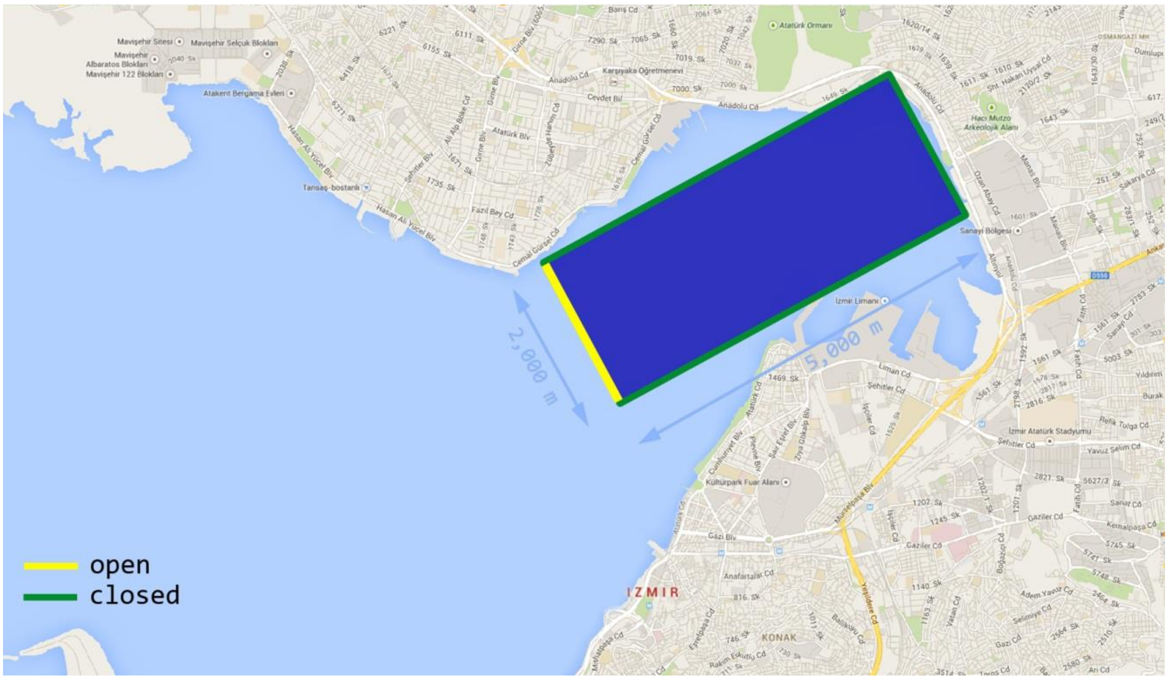


Figure 4.1 Schematization of the "open" computational grid in Izmir Bay (Eastern part of the Aegean Sea).

Based on the available bathymetric data (SRTM-30 database, SIO 2011, Becker et al. 2009), the water depth from near-shore to the offshore boundary increases from 3 to 15 m, resulting in a bottom slope of 0.0024 m/m (i.e. 12 m depth over a horizontal distance of 5,000 m).

The ELV-EQS tool allows for an assessment including up to 10 meteorological/current alternatives. In this second example, two meteorological/current alternatives are used.

The two dominant wind conditions experienced in Izmir Bay are chosen based on the available meteorological information (Sayin 2003, Deltares 2012) and are assumed to occur during 45% and 55% of the time, respectively. First wind conditions are characterized by a Northerly wind direction (360 degrees) with an average wind speed of 3 m/s at 10 m above the ground. Second wind conditions consist of a Southerly wind direction (180 degrees) with an average wind speed of 3.5 m/s at 10 m above the ground.

[3] *An "open" computational grid consists of 1 closed boundary and 3 open boundaries. An "enclosed" environment consists of 1 open boundary and 3 closed boundaries.*

[4] *See [document] describing how to calculate the rotation of the grid.*

Current velocities are derived from the variable wind conditions. For the present example, we will use a current velocity of 0.05 m/s and 0.02 m/s during the Northerly and Southerly wind conditions, respectively (Deltares 2012).

The ambient water temperature in the Bay ranges from 12 to 26 degrees C, and the ambient salinity reaches 39 ppt (Sayin 2003). In our example, the background water temperature is therefore fixed at 20 degrees C and the ambient salinity at 39 ppt (above pycnocline). Furthermore, the concentration of suspended solids is derived from Bizsel and Uslu (2000) with an average value of 22 mg/L (i.e. 22 g/m^3).

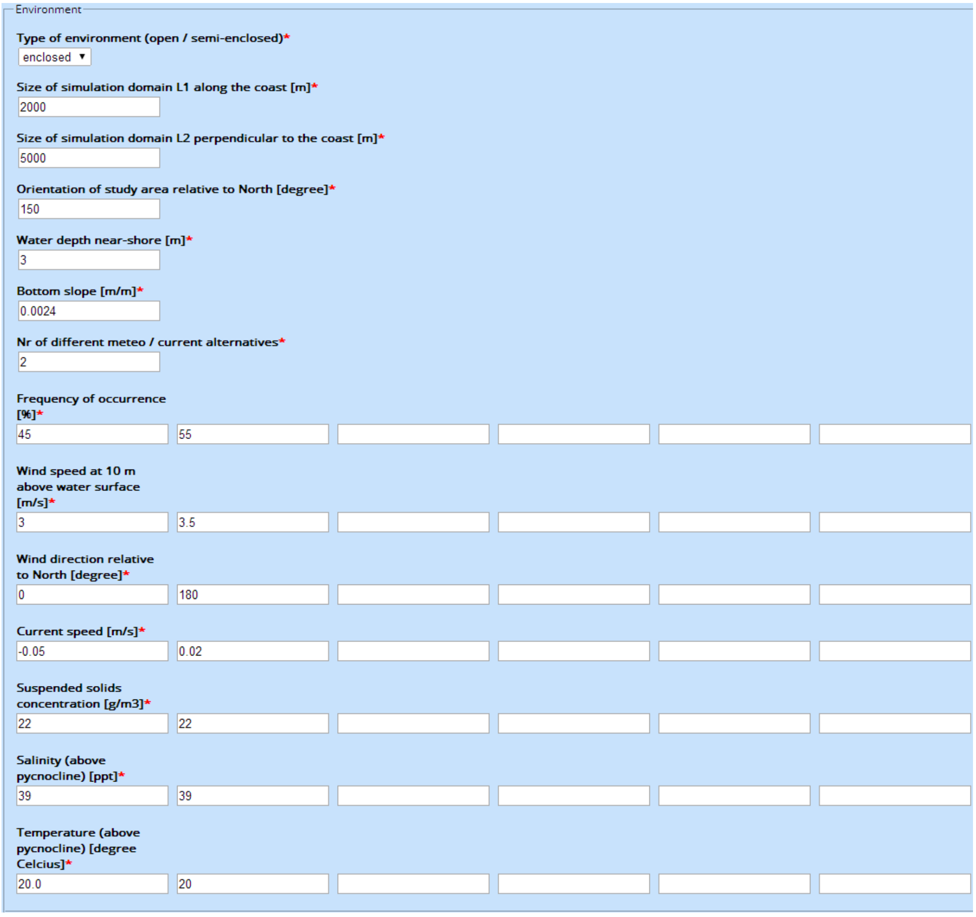
All the values relevant to the environment description are summarized in Table 4.1.

Table 4.1 Properties of the environment

Name	Value	
Study area		
Type of environment	enclosed	
Size of simulation domain L1 along the coast	2,000 m	
Size of simulation domain L2 perpendicular to the coast	5,000 m	
Orientation of study area relative to North	150 degrees	
Water depth near-shore	3 m	
Bottom slope	0.0024 m/m	
Meteo/current alternatives		
Number of different meteo/current alternatives	2	
	North	*South*
Frequency of occurrence	45%	55%
Wind speed at 10 m above water surface	3 m/s	3.5 m/s
Wind direction relative to North	0 degrees	180 degrees
Current speed[5]	-0.05 m/s	0.02 m/s
Receiving water characteristics		
Suspended solids concentration	22 g/m^3	
Salinity (above pycnocline)	39 ppt	
Temperature (above pycnocline)	20 degrees C	

After starting the tool, the user can enter these values in the relevant fields, as shown in Figure 4.2.

[5] *The current speed can be positive or negative, depending on the direction of the wind relative to the orientation of the computational domain. Please refer to (GUID) for more details.*


Environment

Type of environment (open / semi-enclosed)*
enclosed

Size of simulation domain L1 along the coast [m]*
2000

Size of simulation domain L2 perpendicular to the coast [m]*
5000

Orientation of study area relative to North [degree]*
150

Water depth near-shore [m]*
3

Bottom slope [m/m]*
0.0024

Nr of different meteo / current alternatives*
2

Frequency of occurrence [%]*	45	55
Wind speed at 10 m above water surface [m/s]*	3	3.5
Wind direction relative to North [degree]*	0	180
Current speed [m/s]*	-0.05	0.02
Suspended solids concentration [g/m3]*	22	22
Salinity (above pycnocline) [ppt]*	39	39
Temperature (above pycnocline) [degree Celcius]*	20.0	20

Figure 4.2 Definition of the receiving water characteristics in the ELV-EQS tool for Case 2.

4.1.2 Discharge description

The location of the discharge is chosen along the closed longitudinal side, close to the coastline (Figure 3.1). It is located in the longitudinal middle of the grid (X1=1,000 m), and 350 m away for the border of the domain (X2=350 m). Additionally, the discharge is located at the surface of the water column (depth=0.0 m).

In the following, we consider a fresh water discharge containing the simulated pollutant (total mercury). Salinity is equal to 0.0 ppt, while the water temperature of the discharge is fixed at 20 degrees C. Furthermore, it is assumed that the water discharged does not contain particles. Assuming a flow rate of 15 m^3/h (i.e. 0.25 m^3/s) and a load of 1 g/s of the simulated pollutant, the concentration of the simulated pollutant is then 4 g/m^3. Besides, we assume that the discharge occurs from a pipe with a diameter of 0.2 m.

All the values relevant to the discharge characteristics are summarized in Table 4.2.

Table 4.2 Properties of the discharge

Name	Value
Position of discharge along the coast (X1)	1,000 m
Position of discharge from the coast (X2)	350 m
Position of discharge from water surface (depth)	0.0 m
Discharge rate	15 m^3/h
Discharge pipe opening diameter	0.2 m
Discharge temperature	20 degrees C
Discharge salinity	0.0 ppt
Discharge concentration-chemical of concern	4 g/m^3
Discharge concentration of suspended solids	0.0 g/m^3

The user can now enter these values in the relevant fields of the ELV-EQS tool, as shown in Figure 4.3.

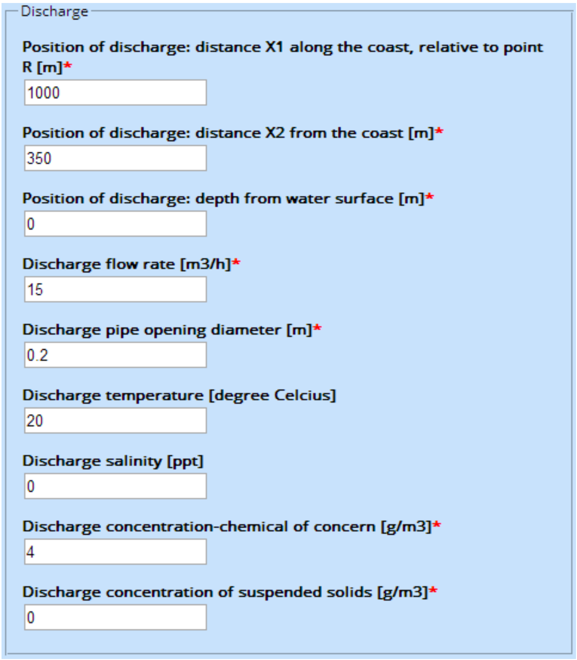


Figure 4.3 Definition of the discharge characteristics in the ELV-EQS tool for Case 2.

4.1.3 Substance properties

In this example, we focus on the discharge of total mercury. For mercury, there is no significant process which effectively removes mercury from the aquatic environment. Metals do not undergo decay, and (GUID) recommends neglecting the settling of the particulate fraction to the sea floor. Therefore, a decay rate of 0.0 d^{-1} is selected for mercury.

In the ELV-EQS tool, a partition coefficient should be specified if the relevant EQS is defined for the dissolved fraction of the substance only (as it is the case for mercury). As discussed in Deltares (2012), the high suspended sediment value causes 90% of mercury to be in the particulate phase. Therefore, the partition coefficient for this substance is 437 m^3/kg (Deltares 2012).

For sake of simplicity, a nil background concentration of total mercury (0.0 g/m^3) is assumed.

In addition, according to the Directive on Environmental Quality Standards (Directive 2008/105/EC, EC 2008), daughter directive of the Water Framework Directive, the maximum allowable concentration (MAC) of mercury and its compounds equals 0.07 µg/L, and the annually average (AA) concentration of mercury and its compounds should not exceed 0.05 µg/L. These EQSs apply to mercury in so-called "other surface waters", and refer to the dissolved fraction of mercury only.

We note that EU guidance document (EC 2010) asks for explicit consideration of separate EQS-MAC and AA-EQS mixing zones, in particular if EQS-MAC is defined. In some European countries, EQS-MAC mixing zone is substantially smaller than EQS-AA mixing zone (approx. 2.5%). However, in the present case, the sizes of the mixing zones for the maximum allowable concentration and the annually averaged concentration are assumed to be identical and equal to 500 m.

Because the ELV-EQS tool is a so-called “rapid assessment tool”, it should adopt a worst-case approach: the simplifications of the tool should never lead to the acceptance of a discharge that would have been rejected in a more detailed assessment. For that reason, we use a safety factor for fate and transport calculation (Deltares 2012). Its value is fixed to 2.

Values describing the properties of the substance discharged are summarized in Table 4.3.

Table 4.3 Properties of the substance

Name	**Value**
Name of the substance	Total mercury
Substance Decay rate	0.0 d^{-1}
Substance Partition Coefficient	437 m^3/kg
Background concentration	0.0 g/m^3
EQS-MAC (maximum allowable concentration)	0.07 µg/L (=7 x 10^{-5} g/m^3)
MAC allowable mixing zone	500 m
EQS-AA (annually averaged concentration)	0.05 µg/L (=5 x 10^{-5} g/m^3)
AA allowable mixing zone	500 m
Safety factor for fate and transport calculation	2

The user can now enter those values in the relevant fields of the ELV-EQS tool, as shown in Figure 4.4.

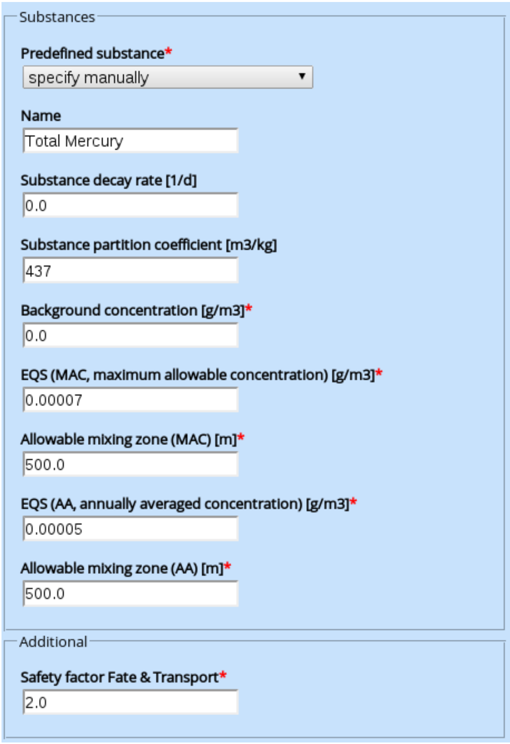


Figure 4.4 Definition of the substance properties in the ELV-EQS tool for Case 2.

Note that it is also possible to select this substance from the list of predefined substances in the dropdown menu. In that case the name, decay rate and partition coefficient do not have to be entered manually.

4.2 Computation

At this point, if you wish to save your input data, use the "Save" button to store all the input information into a text file. Later, you can simply load the text file into the ELV-EQS tool by first selecting the file (using the "Browse" button) and then loading it into the webpage (using the "Load" button), as illustrated in Figure 4.5.

Figure 4.5 Importing input from a saved scenario. Select "Choose File" to browse for an existing saved file. Once chosen, the file name appears next to the button. Select "Load" to load the input data into the ELV-EQS tool.

When all the (correct) information is supplied to the ELV-EQS tool, the "case" can be submitted to the computational core, which will then display the results after a quick computation.

For that purpose, click the button "Submit" at the bottom of the webpage, as shown in Figure 4.6.

Figure 4.6 Submit your case to the computational core to obtain the results.

4.3 Results

After the case has been submitted and the computations have been performed, the webpage displays a page containing the results of the simulation (Figure 4.7). These are presented in a tabular format, showing the annual mean and maximum concentrations of the chemical of concern (here total mercury) at an increasing distance from the source (from 0 to 2,000m).

Distance from pipe [m]	Maximum concentration [g/m3]	Mean concentration [g/m3]
0.	8.000000E+00	8.000000E+00
10.	5.596848E-05	5.563260E-05
20.	3.659202E-05	3.537170E-05
30.	2.825806E-05	2.819019E-05
40.	2.337099E-05	2.315690E-05
50.	2.007700E-05	2.002240E-05
60.	1.776213E-05	1.769873E-05
70.	1.644754E-05	1.641955E-05
80.	1.521248E-05	1.519675E-05
90.	1.403870E-05	1.397926E-05
100.	5.187665E-07	3.802241E-07
200.	3.521806E-07	2.685611E-07
300.	3.163603E-07	2.153027E-07
400.	2.931665E-07	1.844618E-07
500.	2.768122E-07	1.600526E-07
600.	2.653628E-07	1.485556E-07
700.	2.575729E-07	1.441756E-07
800.	2.528344E-07	1.415207E-07
900.	2.502184E-07	1.400551E-07
1000.	2.329938E-07	1.305023E-07
1200.	1.938848E-07	1.088556E-07
1400.	1.666005E-07	9.370878E-08
1600.	1.470133E-07	8.304580E-08
1800.	1.312984E-07	7.616884E-08
2000.	1.190405E-07	6.947558E-08

Figure 4.7 Results page showing the calculated maximum and averaged concentration at several distances from the source of the discharge.

In addition, the EQS, the size of the mixing zone, the concentration at the edge of the mixing zone, and a compliance check are summarized in a table for the maximum and the annual mean concentrations (Figure 4.8). This allows the user to quickly assess whether or not the discharge is permitted, and if not, where the threshold is exceeded.

description	Maximum concentration [g/m3]	Mean concentration [g/m3]
EQS	7.000000E-05	5.000000E-05
defined mixing zone	5.000000E+02	5.000000E+02
concentration at edge of defined mixing zone	2.768122E-07	1.600526E-07
discharge permitted?	YES	YES

Figure 4.8 Summary table indicating the results of the compliance check.

In this second example, the compliance with the EQS for maximum (0.7 µg/L) and annual mean concentration (0.5 µg/L) of total mercury are not exceeded at the edge of their respective mixing zones (500 m for both). Maximum and annual mean concentrations are not equal in this case, since the scenario consists of two wind/current alternatives. Nonetheless, the discharge is still permitted.

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