**BETR-QWASI-LU**

**A spatially resolved QWASI model for vertically layered coastal waters**

**with Uncertainty Analysis**

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# MODELING STRUCTURE

(1) Upper Ocean

(3) Sediment

(2) Lower Ocean

Figure 1. Compartments of BETR-QWASI-L

# INPUT FILES

## Chemical Database

This is a text file to input chemical properties.

Location: …/Chemicals/

The file name should be stated in the run-file as a string with the variable name: “chemdata”.

The default chemical database file is named “chemicals\_QWASI.txt”.

Table 1. Chemical database components

|  |  |
| --- | --- |
| Name of the variable | Description |
| ID | Unique database identifier |
| T0 | Standard temperature (K) |
| molmass | Molar mass (g/mol) |
| logKaw | Partitioning coefficient air-water (dimensionless) |
| logKow | Partitioning coefficient octanol-water (dimensionless) |
| logKoa | Partitioning coefficient octanol-air (dimensionless) |
| halflife\_air | Halflife in air (h) |
| halflife\_ocean | Halflife in ocean (h) |
| halflife\_sediment | Halflife in sediment (h) |
| DUoa | Internal energy of phase change octanol-air (J/mol) |
| DUow | Internal energy of phase change octanol-water (J/mol) |
| EA\_air | Activation energy in air (J/mol) |
| EA\_ocean | Activation energy in ocean (J/mol) |
| EA\_sediment | Activation energy in sediment (J/mol) |
| notes | Comments and descriptions |

## Control File

This is a text file to control the simulation options.

Location: …/Control/

The file name should be stated in the run-file as a string with the variable name: “contfile”.

The default control file is named “control\_QWASI.txt”.

The contents of “control\_QWASI.txt”:

# File with options for a BETR-Research model

# Format:

# comment-lines start with

# first column: option\_name

# second column: option\_value

# delimiter: whitespace

#

# make D-matrix output in 2 different formats

dumpDmatrices 0

dumpDmatricesTxt 0

An option value of 0 turns the option off while an option value of 1 turns the option on.

Current options that can be controlled within the control file:

dumpDmatrices

When this option is on (option\_value = 1), the list of matrices that contains all the D values for the current model run are dumped into a file (filename = matrixdump.cpk) using the pickle module. This file contains the data of a list of sparse matrices. The file can be unpickled in a Python script to reload the list of D-value matrices. The pickle dump is done at the model initialization step. So, it is possible to produce the D-value matrices and write them into a file without running a simulation. This can be achieved by initializing the Model class in the run-file, but not running the further code that solves the model.

dumpDmatricesTxt

When this option is on (option\_value = 1), the list of matrices that contains all the D values for the current model run are written into a text file (filename = matrixdump.txt). This is done at the model initialization step. So, it is possible to produce the D-value matrices and write them into a text file without running a simulation. This can be achieved by initializing the Model class in the run-file but not running the further code that solves the model.

## Emissions Data Files

Emissions data files are text files that provide the temporal and spatial distribution of the chemical emission to the model. They are located in the folder “Emissions”.

Format:

[m] [r] [c1] [c2] [c3] [val1] [val2] [val3]

where

|  |  |
| --- | --- |
| m | number of month (starts from 1) |
| r | cell number |
| c1 | compartment 1 (upper ocean) (enter the value 1) |
| c2 | compartment 2 (lower ocean) (enter the value 2) |
| c3 | compartment 3 (sediment) (enter the value 3) |
| val1 | emissions into upper ocean in cell r during month m (mol/h) |
| val2 | emissions into lower ocean in cell r during month m (mol/h) |
| val3 | emissions into sediment in cell r during month m (mol/h) |

Month values (m) from 1 to 12 will define emissions for a complete year. If the simulation will proceed longer than a year, the same values will be repeated. Multi-year simulations with annually varying emissions data can be described by either defining emissions for each month of the simulation in a single emissions file, or by creating separate emissions data files for each year and storing them in the folder “Emissions/annual/ “(this would require setting up the run-file in a specific way so that multiple yearly simulations are conducted in series). For steady-state runs this data column is ignored.

## Compartments File

This is a text file that lists the compartments considered by the model.

Location: …/Environment/

The file name should be stated in the run-file as a string with the variable name: “compfile”.

The default compartments file is named “compartments\_QWASI.txt”.

For each compartment, the variable name used in the code to assign temperature, contaminant half-life and contaminant’s activation energy values associated with that compartment are also listed. Explanations are given in the comments section at the top of the file.

The contents of “compartments\_QWASI.txt” are given and described below:

#

# compartments\_QWASI.txt contains the compartments considered by the model.

# It is possible to insert new compartments or comment out existing ones.

# Lines starting with '''#''' are comments. Lines are either comments or data.

# Beware of empty lines (particularly at the end of the file) !

#

# The first non-comment line contains the names of the variables.

# These names are used in the code only change them if you know what you

# are doing !

#

# Columns:

#

# ID : integer number of the compartment

# name : a description must be valid Python dictionary key (no spaces etc.)

# temp\_variable : the variable name that contains the temperature

# of the compartment (in seasonal\_QWASI.txt)

# halflife\_variable : variable name that contains the halflife of chemicals

# in the compartment : (in chemicals\_QWASI.txt)

# EA\_variable : variable name that contains activation energy of chemicals

# in the compartment : (in chemicals\_QWASI.txt)

#

ID name temp\_variable halflife\_variable EA\_variable

1 upper\_ocean tupperocean halflife\_ocean EA\_ocean

2 lower\_ocean tlowerocean halflife\_ocean EA\_ocean

3 sediment tsed halflife\_sediment EA\_sediment

Table 2. Compartment specifications defined in the compartments input file

|  |  |
| --- | --- |
| Name of the variable\* | Description |
| ID | Compartment number (integer number identifying the compartment) |
| name | Compartment name (must be a valid Python dictionary key) |
| temp\_variable | Variable name that contains the temperature of the compartment (its value should be provided in the seasonal parameters file) |
| halflife\_variable | Variable name that contains the halflife of chemicals in the compartment (its value should be provided in the chemical database) |
| EA\_variable | Variable name that contains activation energy of chemicals in the compartment (its value should be provided in the chemical database) |

**\***: These names are used in the code.

## Constant Environmental Parameters File

This is a text file that specifies the constant environmental parameters (environmental parameters that do not change with time).

Location: …/Environment/

The file name should be stated in the run-file as a string with the variable name: “constparfile”.

The default constant environmental parameters file is named “const\_parameters\_QWASI\_2BasinIzmit.txt”.

At the beginning of the file, lines starting with “#” are comments. Comment lines must form a continuous block at the beginning of the file. The last comment line must contain the names of the variables that are used in the code. The data has to start in the following line.

File structure, syntax and the variable names for the environmental parameters are described as comments at the beginning of the default file “const\_parameters\_QWASI\_1.txt”.

Table . Environmental parameters defined in the constant environmental parameters file

|  |  |
| --- | --- |
| Name of the variable\* | Description |
| CELL | Cell number |
| fp1 | Volume fraction of particles in upper ocean |
| fp2 | Volume fraction of particles in lower ocean |
| fw7 | Volume fraction of pore water in sediment |
| fs7 | Volume fraction of solids in sediment |
| focp1 | Mass fraction of organic carbon in particles in upper ocean |
| focp2 | Mass fraction of organic carbon in particles in lower ocean |
| focs7 | Mass fraction of organic carbon in solids in sediment |
| rhop12 | Density of particles in air (kg/m3) |
| rho45 | Density of water (kg/m3) |
| rhop45 | Density of particles in water (kg/m3) |
| rhos7 | Density of solids in sediment (kg/m3) |
| scavrain | Rain scavenging ratio |
| scavsnow | Snow scavenging ratio |
| A | Total surface area (m2) |
| perc5 | Fraction of surface covered by coastal water |
| partsett | particle settling (upper ocean) (m/h) |
| h7 | Average sediment compartment depth (m) |
| diff7water | Sediment-water diffusion mass transfer coefficient (m/h) |
| seddep | Sediment deposition (lower ocean) (m/h) |
| sedresup | Sediment resuspension (m/h) |
| sedburial | Sediment burial (m/h) |
| mtc25air | Air side air-coastal water mass transfer coefficient (m/h) |
| mtc25water | Water side air-coastal water mass transfer coefficient (m/h) |

**\***: These names are used in the code.

## Seasonal Environmental Parameters File

This is a text file that specifies the seasonal environmental parameters (environmental parameters that change with time).

Location: …/Environment/

The file name should be stated in the run-file as a string with the variable name: “seasparfile”.

The default constant environmental parameters file is named “seasonal\_parameters\_QWASI\_2BasinIzmit.txt”.

At the beginning of the file, lines starting with “#” are comments. Comment lines must form a continuous block at the beginning of the file. The last comment line must contain the names of the variables that are used in the code. The data has to start in the following line.

File structure, syntax and the variable names for the environmental parameters are described as comments at the beginning of the default file “seasonal\_parameters\_QWASI\_1.txt”.

Table . Environmental parameters defined in the seasonal environmental parameters file

|  |  |
| --- | --- |
| Name of the variable\* | Description |
| CELL | Cell number |
| TS | Timestep. (Usually corresponds to a month. Values from 1 to 12 will define parameter values for a complete year. If the simulation will proceed longer than a year, the same values will be repeated.) |
| tair2 | Temperature of lower air [K] |
| tupperocean | Temperature of the upper ocean (K) |
| tlowerocean | Temperature of the lower ocean (K) |
| tsed | Temperature of the sediment compartment (K) |
| h1 | Average upper ocean compartment depth (m) |
| h2 | Average lower ocean compartment depth (m) |
| perc8 | Fraction of ocean covered by sea ice (-) |
| G | Water outflow rate from the ocean compartment (m3/h) |

**\***: These names are used in the code.

## Input Files for Environmental Flows

These text files specifies water flows between corresponding ocean compartments in neighboring cells and between lower and upper ocean compartments in the same cell.

Location: …/Flows/

The multiple flow files that are to be used in a simulation should be placed in a subfolder and the name of this subfolder should be stated in the run-file as a string with the variable name: “flowdirectory”.

The default flow files are placed in the folder named “QWASI\_2BasinIzmit\_Layered”.

At the beginning of the file, lines starting with “#” are comments. Comment lines must form a continuous block at the beginning of the file. The last comment line must specify the compartment where the flow is originated and the compartment where the flow is going in. This is done by writing down the character “#” followed by the compartment number where the flow is originated (from) and the compartment number where the flow is going in (to) separated by a space character. For example, the flow file that specifies flows from an upper ocean compartment in a cell to another upper ocean compartment in another cell must have the following line as the last comment line:

#1 1

Following the comment lines, the flow quantities must be entered in units of m3/h for each timestep (month of year). Twelve flow values in a single line will define parameter values for a complete year. If the simulation will proceed longer than a year, the same values will be repeated.

The format is as follows:

[FROM] [TO] [val1] [val2] [val3] [val4] ... [val12]

where

|  |  |
| --- | --- |
| FROM | cell number where the flow is coming from |
| TO | cell number where the flow is going to |
| val1 | flow quantity from FROM to TO in month 1 (m3/h) |
| val2 | flow quantity from FROM to TO in month 2 (m3/h) |
| val3 | flow quantity from FROM to TO in month 3 (m3/h) |
| val4 | flow quantity from FROM to TO in month 4 (m3/h) |
| val5 | flow quantity from FROM to TO in month 5 (m3/h) |
| val6 | flow quantity from FROM to TO in month 6 (m3/h) |
| val7 | flow quantity from FROM to TO in month 7 (m3/h) |
| val8 | flow quantity from FROM to TO in month 8 (m3/h) |
| val9 | flow quantity from FROM to TO in month 9 (m3/h) |
| val10 | flow quantity from FROM to TO in month 10 (m3/h) |
| val11 | flow quantity from FROM to TO in month 11 (m3/h) |
| val12 | flow quantity from FROM to TO in month 12 (m3/h) |

## Processes File

This is a text file that specifies the fate and transport processes considered by the model. This is done by listing the name of the method of the class process coded in the file /PY/processes.py. The compartments that need to be present in order to consider the particular process also need to be listed.

Location: …/Processes/

The file name should be stated in the run-file as a string with the variable name: “procparfile”.

The default processes file is named “processes\_QWASI.txt”.

The contents of “processes\_QWASI.txt”:

#

# processes\_QWASI.txt contains the processes considered by the QWASI model.

# Processes can be commented out and new processes can be added.

#

# Lines starting with '''''''#''''''' are comments. Lines are either comments or data.

# Beware of empty lines (particularly at the end of the file) !

#

# The first column contains the name of the process. This string has to be

# valid as function-name in Python (starts with letter, contains letters

# numbers, underscores).

#

# The following columns contain a list of the compartments that need

# to be present to consider that process.

#

#process\_name compartments

betr\_degradation 1 2 3

betr\_advectiveloss 1 2 3

betr\_diff\_loss 1

betr\_ocean\_partsett 1 2

betr\_sediment\_ocean\_resusp 3 2

betr\_ocean\_sediment\_deposit 2 3

betr\_ocean\_sediment\_diff 2 3

Table . The methods of the process class that define the fate and transport processes in the BETR-QWASI.

|  |  |  |
| --- | --- | --- |
| Name of the method\* | The fate/transport process | Compartments involved |
| betr\_degradation | Degradation loss from the compartment | upper ocean, lower ocean, sediment |
| betr\_advectiveloss | Advective loss from the compartment | upper ocean and lower ocean (advective loss by water flow), sediment (burial) |
| betr\_diff\_loss | Diffusive loss from the compartment | Diffusive loss from upper ocean to air |
| betr\_ocean\_partsettl | Transfer by particle settling from upper ocean to lower ocean | upper ocean, lower ocean |
| betr\_sediment\_ocean\_resusp | Transfer by particle resuspension from sediment to ocean | sediment, lower ocean |
| betr\_ocean\_sediment\_deposit | Transfer by particle deposition from ocean to sediment | lower ocean, sediment |
| betr\_ocean\_sediment\_diff | Diffusive transfers between ocean and sediment | lower ocean, sediment |

**\***: These names are used in the code when defining the process class.

## Parameters for the Differential Equation Solver

This text file provides the parameters for the differential equation solver.

Location: …/Solver/

The file name should be stated in the run-file as a string with the variable name: “solvfile”.

The default processes file is named “solvparams\_default.txt”.

The contents of “solvparams\_default.txt”:

# Parameters for the solver of BETR-Research

# integname: default = vode

# method: adams or bdf

# maxsubsteplength = 730

# atol: default = 3E-014

# rtol: default = 1e-6. (should be < 1e-4)

# order: default = 5

# with\_jacobian: default = 1

# nsteps: default = 1000

integname vode

method adams

maxsubsteplength 730

atol 3E-014

rtol 0.000001

order 5

with\_jacobian 1

nsteps 5000

There are several versions of the solver parameters file in the …/Solver/ folder. The main difference between these versions is in the tolerance parameter values. They can be opted to be used in certain situations (e.g. when more accurate results are required, when the solver with the default parameters failed to produce a result).

Table 6. Versions of the solver parameters file available in the folder …/Solver/

|  |  |  |
| --- | --- | --- |
| Name of the file | Main parameters | Description |
| solvparams\_default.txt | method adams  atol 3E-014  rtol 0.000001 | The default solver parameters. |
| solvparams\_strict1.txt | method adams  atol 3e-16  rtol 1e-8 | Lower tolerance values for more accurate results. |
| solvparams\_strict2.txt | method adams  atol 3e-18  rtol 1e-10 | Lower tolerance values for more accurate results. |
| solvparams\_strict3.txt | method adams  atol 3e-20  rtol 1e-12 | Lower tolerance values for more accurate results. |
| solvparams\_unstab1adams.txt | method adams  atol 3e-10  rtol 1e-4 | Higher tolerance values. To be used when the solver fails with the default values. |
| solvparams\_unstab1bdf.txt | method bdf  atol 3e-10  rtol 1e-4 | Higher tolerance values. To be used when the solver fails with the default values. |
| solvparams\_unstab2adams.txt | method adams  atol 3e-6  rtol 1e-2 | Higher tolerance values. To be used when the solver fails with the default values. |
| solvparams\_unstab2bdf.txt | method bdf  atol 3e-6  rtol 1e-2 | Higher tolerance values. To be used when the solver fails with the default values. |

## Initial Conditions

This text file provides the initial conditions at the start of the simulation. More specifically, it provides the mass of contaminant in each compartment in each region at time 0.

Location: …/Solver/

The default processes file is named “initial\_default.txt”. If this file is used, it is not needed to specify it when calling the solver. Otherwise, the file name should be stated in the run-file when calling the method “update\_solver” (as the third argument or with the keyword: initfile).

The contents of “initial\_default.txt”, which contains the description of the required format (as comments starting with #) is given below:

## inital conditions for BETR-Research

## first column: region-id

## second column: compartment-id

## third column: amount in mol

## if this file contains no values, an uncontaminated environment at t=0 is assumed.

##

#1 1 1e-6

#1 2 1e-6

#1 3 1e-6

## Time Step and Period Values for Dynamic Simulations

This text file connects the period and step values for dynamic simulation by specifying a set of time offset values in hours.

Location: …/Solver/

The default processes file that defines one-month time steps and a one-year period is provided as stepping\_default.txt. If this file is used, it is not needed to specify it when calling the solver. Otherwise, the file name should be stated in the run-file when calling the method “update\_solver” (as the first argument or with the keyword: stepfile).

The contents of “stepping\_default.txt”, which contains the description of the required format (as comments starting with #) is given below:

# stepping.txt connects period and step (usually year and month)

# to an actual time-offset (from t0).

#

# The format is as whitespace-seperated list of:

# duration(hours)\_of\_step\_1 duration\_of\_step2 ...... duration\_of\_last\_step

#

# The typical (dynamic) BETR-Global entry would be

# 730 730 730 730 730 730 730 730 730 730 730 730

#

# For steady-state evaluations of the model, this file is not used.

#

#

730 730 730 730 730 730 730 730 730 730 730 730

# Intra-Region Transfer Processes

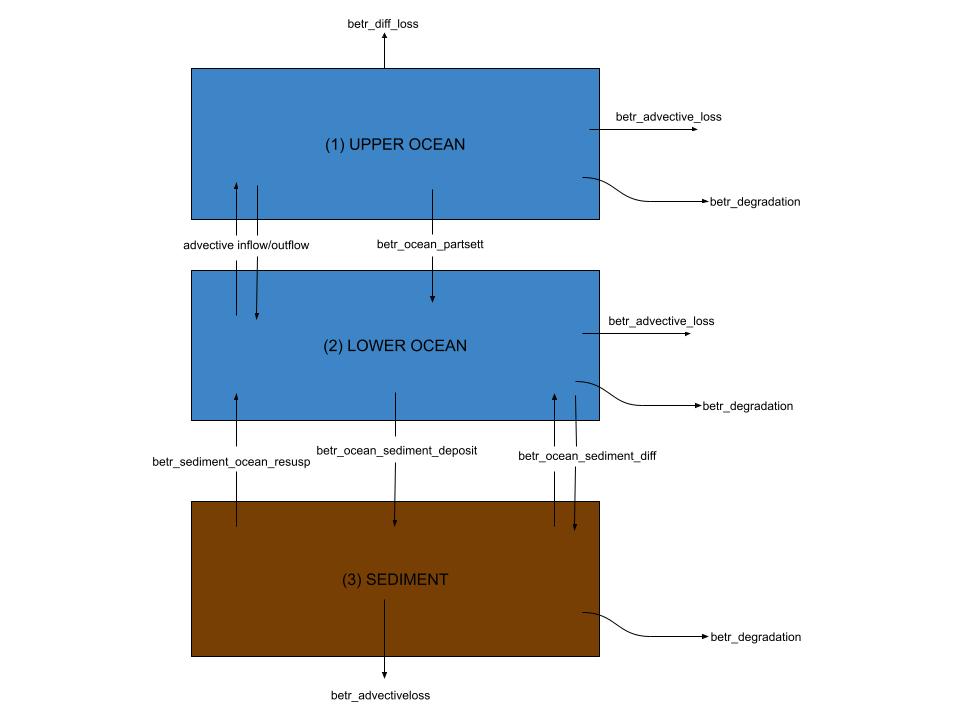


Figure . Intra-region transfer processes considered and the methods of the “process“ class that calculate D-values for these procesess

Intra-region transfer processes include transfer processes between the compartments in a region and the loss processes (i.e. degradation, advective losses, diffusive losses).

Module “processes” in the folder …/PY/ contains these process definitions and calculates D-values (mol/h/Pa) for them. It contains the definition of a class, called “process” that contains the process descriptions as methods. The names of these methods are listed in the processes input file (Section 2.8).

Advective inflow/outflow between upper and lower ocean compartments are intra-region transfer processes due to ocean flows between these compartments. However, this intra-region advective processes are dealt with the same way as the other inter-cell environmental flows by defining the flow rates in environmental flow input files.

## betr\_degradation

This method describes the degradation process in all the compartments. Degradation D-value for each compartment (*D*degradation) is calculated as follows:

 (Equation )

where

*Ddegredation* : degradation D-value for each compartment (mol/h/Pa)

*kreac* : first-order reaction rate constant (h-1) (calculated using the half-life value –

**(halflife\_ocean, halflife\_sediment)**

*Vbulk* : bulk volume of the compartment (m3)

*Zbulk* : bulk Z-value for the compartment (mol/ m3/Pa)

## betr\_advective\_loss

### Sediment burial

This method describes the sediment burial process in the sediment compartment. Sediment burial D-value for the sediment compartment (*D*burial) is calculated as follows:

 (Equation )

*Dburial* : sediment burial D-value for the sediment compartment (mol/h/Pa)

*A* : Total surface area (m2) (**A**)

*Uburial* : sediment burial rate (m/h) (**sedburial**)

*Zss*: Z-value for sediment solids (mol/m3/Pa)

### Water outflow

This method describes the water outflow process in the ocean compartment. Water outflow D-value for ocean compartment (*D*adv) is calculated as follows:

 (Equation )

where

*D*adv : water outflow D-value for the ocean compartment (mol/h/Pa)

*G* : water outflow rate from the ocean compartment (m3/h) (**G**)

*Zwbulk* : bulk Z-value for the ocean compartment (mol/m3/Pa)

## betr\_diff\_loss

This method describes the diffusive loss process in the upper ocean compartment to air. Diffusive loss D-value for the upper ocean compartment (*D*difloss) is calculated as follows:

 (Equation )

where

*D*difloss : diffusive loss D-value for the upper ocean compartment (mol/h/Pa)

*A* : total surface area (m2) (**A**)

*ka* : air side mass transfer coefficient on the air/water interface (m/h) **(mtc25air)**

*Za* : 1/(R×T) (R: ideal gas constant (8,314 m3-Pa/mol-K); T: ambient temperature (K))

*kw* : water side mass transfer coefficient on the air/water interface (m/h) **(mtc25water)**

*Zw* : Z-value for the upper ocean water (mol/m3/Pa)

## betr\_ocean\_partsett

This method describes the particle settling process in the upper ocean compartment. The particle settling D-value from the upper ocean compartment to the lower ocean compartment (*Dpartsett*) is calculated as follows:

 (Equation )

where

*Dpartsett* : particle settling D-value for the ocean compartment (mol/h/Pa)

*A* : Total surface area (m2) (**A**)

*Upartsett*: particle settling rate (m/h) **(partsett)**

*Zss*: Z-value for suspended solids (mol/m3/Pa)

## betr\_sediment\_ocean\_resusp

This method describes the sediment resuspension process in the ocean compartment. Sediment resuspension D-value for the ocean compartment (*D*resusp) is calculated as follows:

 (Equation )

where

*Dresusp* : sediment resuspension D-value for the ocean compartment (mol/h/Pa)

*A* : Total surface area (m2) (**A**)

*Ur*: sediment resuspension rate (m/h) **(sedresup)**

*Zs*: Z-value for sediment (mol/m3/Pa)

## betr\_ocean\_sediment\_deposit

This method describes the sediment deposition process in the lower ocean compartment. Sediment deposition D-value for the lower ocean compartment (*D*deposit) is calculated as follows:

 (Equation )

where

*D*deposit : sediment deposition D-value for the lower ocean compartment (mol/h/Pa)

*A* : Total surface area (m2) (**A**)

*Udep* :sediment deposition rate (m/h) **(seddep)**

*Zss* : Z-value for suspended solids (mol/m3/Pa)

## betr\_ocean\_sediment\_diff

This method describes the diffusion exchange process between the lower ocean and sediment compartments. Diffusive exchange process D-value between the lower ocean and sediment compartments (*D*diff) is calculated as follows:

 (Equation )

where

*D*diff : diffusive exchange D-value between the lower ocean and sediment compartments (mol/h/Pa)

*A* : total surface area (m2) (**A**)

*kw-s* : sediment-water diffusion mass transfer coefficient (m/h) **(diff7water)**

*Zw* : Z-value for the lower ocean water (mol/m3/Pa)

# Compartment Volumes

Module “volumes” in the folder …/PY/ calculates the compartment and sub-compartment volumes (m3). It contains the definition of a class, called “Volumes” that contains the volume descriptions for each compartment as methods. The methods and the volumes they calculate are explained below.

## V1 (Upper Ocean Compartment) and V2 (Lower Ocean Compartment)

These two method describes the bulk volumes of the ocean compartments, the volumes of suspended solids in the ocean compartments, and the volumes of water in the ocean compartments.

Bulk volume of the ocean compartments (*Voceanbulk)* is calculated as follows:

 (Equation )

where

*Voceanbulk* : bulk volume of the ocean compartment (m3)

*A* : total surface area (m2) **(A)**

*fAocean*: fraction of surface covered by coastal water **(perc5)**

*h*: average ocean compartment depth (m) **(h1 or h2)**

Volume of suspended solids in the ocean compartment (*Vsussed)* is calculated as follows:

 (Equation )

where

*Vsussed* : volume of suspended solids in the ocean compartment (m3)

*Voceanbulk* : bulk volume of the upper ocean compartment (m3)

*fp* : volume fraction of particles in ocean water **(fp1 or fp2)**

Volume of water in the ocean compartment (*Vwater)* is calculated as follows:

 (Equation )

where

*Vwater* : volume of the water in the ocean compartment (m3)

*Voceanbulk* : bulk volume of the ocean compartment (m3)

*Vsussed* : volume of suspended solids in the ocean compartment (m3)

## V3 (Sediment Compartment)

This method describes the bulk volume of the sediment compartment, the volume of water in the sediment compartment, and the volume of solids in the sediment compartment.

Bulk volume of the sediment compartment (*Vsedbulk)* is calculated as follows:

 (Equation )

where

*Vsedbulk* : bulk volume of the sediment compartment (m3)

*A* : total surface area (m2) **(A)**

*fAocean*: fraction of surface covered by coastal water **(perc5)**

*h7* : average sediment compartment depth (m) **(h7)**

Volume of water in the sediment compartment (*Vwater)* is calculated as follows:

 (Equation )

where

*Vwater* : volume of water in the sediment compartment (m3)

*Vsedbulk* : bulk volume of the sediment compartment (m3)

*fsedwater* : volume fraction of pore water in sediment **(fw7)**

Volume of solids in the sediment compartment (*Vsolids)* is calculated as follows:

 (Equation )

*Vsolids* : volume of solids in the sediment compartment (m3)

*Vsedbulk* : bulk volume of the sediment compartment (m3)

*fsedsolids* : volume fraction of solids in sediment **(fs7)**

# Z-Values

Module “zvalues” in the folder …/PY/ calculates the Z-values (mol/m3Pa) for all the compartments and their sub-compartments. It contains the definition of a class, called “Zvolumes” that contains the Z-value descriptions for each compartment as methods. The methods and the Z-values they calculate are explained below.

## Z1 and Z2 (Upper Ocean Compartment and Lower Ocean Compartment)

These methods describes the Z-values for water in the ocean compartments, Z-values for suspended sediments in the ocean compartments, Z-value for the air boundary layer over the upper ocean compartment (only Z1) and the bulk Z-values of the ocean compartments.

Z-values for water in the ocean compartment (*Zwater*) is calculated as follows:

 (Equation )

where

*Zoceanwater* : Z-value of ocean water (mol/m3Pa)

*R* : ideal gas constant (8.314 m3Pa/molK)

*T* : temperature of the compartment (K)

*Kaw*: air-water partition coefficient

Z-values for suspended sediment in the ocean compartment (*Zsussed*) is calculated as follows:

 (Equation )

where

*Zsussed* : Z-value of suspended sediment in the ocean compartment (mol/m3Pa)

*Zoceanwater* : Z-value of ocean water (mol/m3Pa)

*Kqw*: suspended sediment - water partition coeffcient

Suspended sediment-water partition coeffcient (*Kqw*) is calculated as follows:

 (Equation 17)

where

*Kqw* : suspended sediment - water partitioning coeffcient

*0.41* : the factor defining the relationship between Kow and the Koc (L/kg)

*Kow*: octanol-water partition coefficient

*focp* : mass fraction of organic carbon in particles in ocean water **(focp1 or focp2)**

 : density of particles in water (kg/m3) **(rhop45)**

Z-value for the bulk ocean (*Zoceanbulk*) is calculated as follows:

 (Equation )

where

*Zoceanbulk*: Z-value of the bulk ocean (mol/m3Pa)

*fp* : volume fraction of particles in ocean water **(fp1 of fp2)**

*Zoceanwater* : Z-value of ocean water (mol/m3Pa)

*Zsussed* : Z-value of suspended sediment in the ocean compartment (mol/m3Pa)

Z-value for the air boundary layer over the upper ocean water (*Zair*) is calculated as follows:

 (Equation )

where

*Zair* : Z-value of air boundary layer over the upper ocean compartment (mol/m3Pa)

*R* : ideal gas constant (8.314 m3Pa/molK)

*T* : temperature of compartment (K)

## Z3 (Sediment Compartment)

This method describes the Z-value for water in the sediment compartment, Z-value for soilds in the sediment compartment, and the bulk Z-value of the sediment compartment.

Z-value for water in the sediment compartment (*Zsedwater*) is calculated as follows:

 (Equation )

where

*Zsedwater* : Z-value of sediment water (mol/m3Pa)

*R* : ideal gas constant (8.314 m3Pa/molK)

*T* : temperature of compartment (K)

*Kaw*: air-water partition coefficient

Z-value for solids in the sediment compartment (*Zsolids*) is calculated as follows:

 (Equation )

where

*Zsolids* : Z-value of solids in sediment (mol/m3Pa)

*Zsedwater* : Z-value of sediment water (mol/m3Pa)

*Ksedw* : solids in sediment - water partitioning coefficient

Solids in sediment - water partitioning coefficient (*Ksedw*) is calculated as follows:

 (Equation 22)

where

*Ksedw* : solids in sediment - water partitioning coefficient

*0.41* : the factor defining the relationship between Kow and the Koc (L/kg)

*Kow*: octanol-water partition coefficient

*focs* : mass fraction of organic carbon in solids in sediment **(focs7)**

 : density of solids in sediment (kg/m3) **(rhos7)**

Z-value for the bulk sediment (*Zsedbulk*) is calculated as follows:

 (Equation )

where

*Zsedbulk* : Z-value of the bulk sediment (mol/m3Pa)

*fw* : volume fraction of pore water in sediment **(fw7)**

*Zsedwater* : Z-value of sediment water (mol/m3Pa)

*fs* : volume fraction of solids in sediment **(fs7)**

*Zsolids* : Z-value of solids in sediment (mol/m3Pa)