BETR-QWASI-LU

A spatially resolved QWASI model for vertically layered coastal waters with Uncertainty Analysis

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April 2022

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ACKNOWLEDGEMENTS

BETR-QWASI-LU has been developed as a part of a research project funded by The Scientific and Technological Research Council of Turkey (TUBITAK) (Project Number: 118Y155).

The source code of BETR-QWASI-LU is based on BETR-Global 4.0 by Matthew MacLeod and Fangyuan Zhao. The Python 3.0 patch of BETR-Global 4.0 by Baron Henderson facilitated the code development.

1. MODELING STRUCTURE

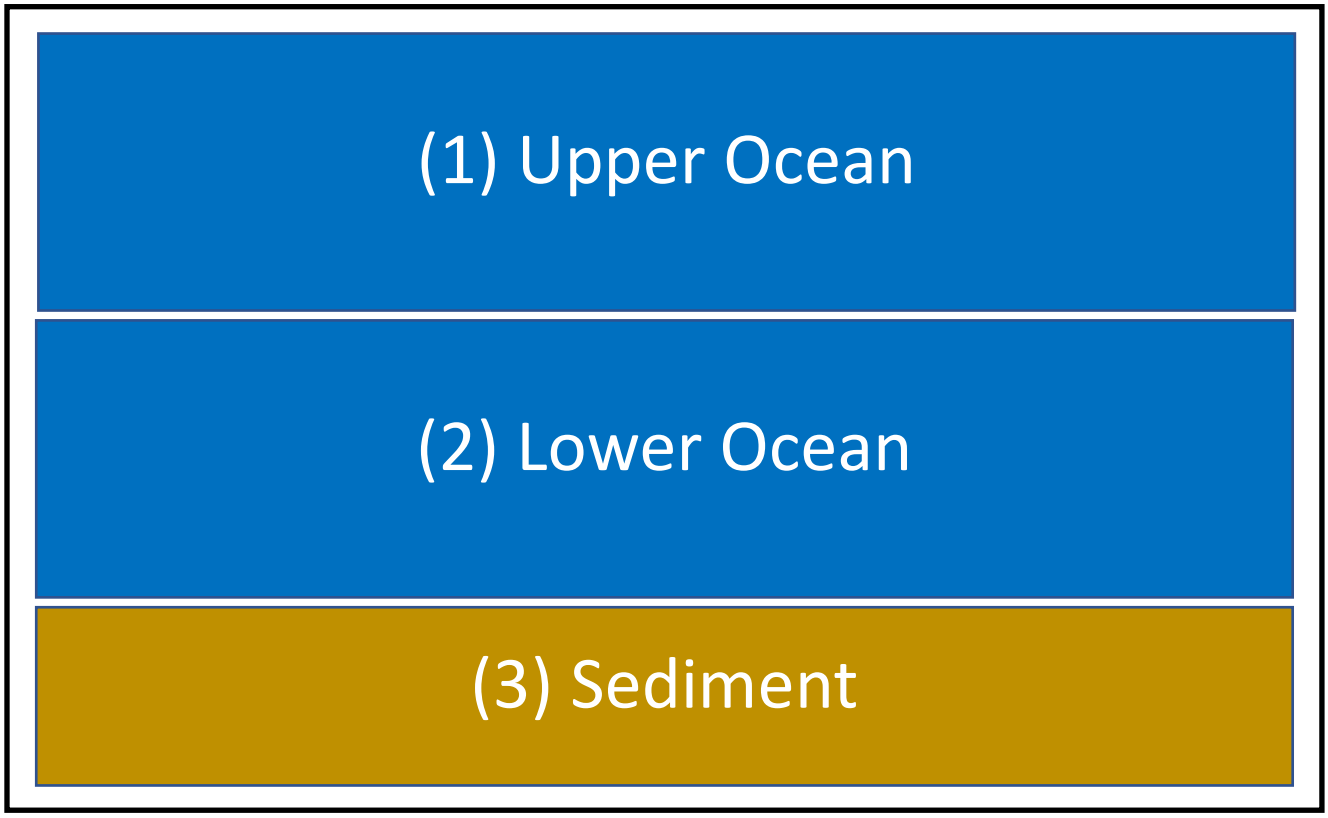

Figure 1. Compartments of BETR-QWASI-L

2. INPUT FILES

2.1. 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

2.2. 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.

2.3. 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.

2.4. 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.

2.5. 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_2BasinIzmit.txt”.

Table 3. 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/m^3)
rho45	Density of water (kg/m^3)
rhop45	Density of particles in water (kg/m^3)
rhos7	Density of solids in sediment (kg/m^3)
scavrain	Rain scavenging ratio
scavsnow	Snow scavenging ratio
A	Total surface area (m^2)
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.

2.6. 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_2BasinIzmit.txt”.

Table 4. 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 (m^3/h)

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

2.7. Input Files for Environmental Flows

These text files specify 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 m^3/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 (m^3/h)
val2	flow quantity from FROM to TO in month 2 (m^3/h)
val3	flow quantity from FROM to TO in month 3 (m^3/h)
val4	flow quantity from FROM to TO in month 4 (m^3/h)
val5	flow quantity from FROM to TO in month 5 (m^3/h)
val6	flow quantity from FROM to TO in month 6 (m^3/h)
val7	flow quantity from FROM to TO in month 7 (m^3/h)
val8	flow quantity from FROM to TO in month 8 (m^3/h)
val9	flow quantity from FROM to TO in month 9 (m^3/h)
val10	flow quantity from FROM to TO in month 10 (m^3/h)
val11	flow quantity from FROM to TO in month 11 (m^3/h)
val12	flow quantity from FROM to TO in month 12 (m^3/h)

2.8. 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 5. 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.

2.9. 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.

2.10. 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
```

2.11. 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
```

3. INTRA-REGION TRANSFER PROCESSES

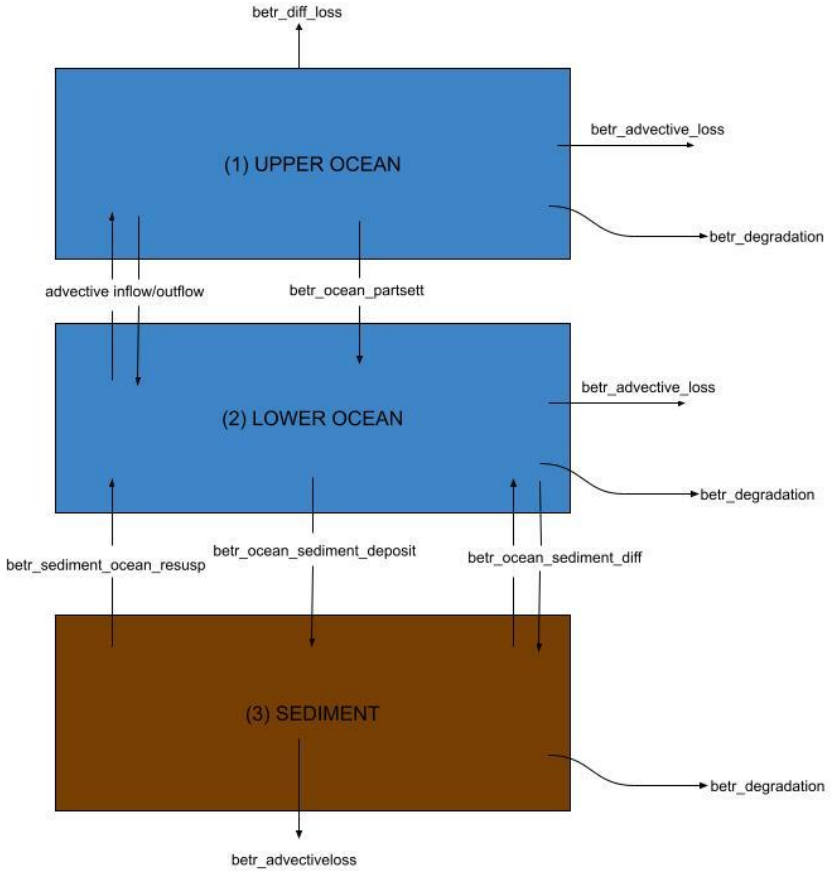

Figure 2. Intra-region transfer processes considered and the methods of the “process“ class that calculate D-values for these procesess

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.

3.1. betr_degradation

This method describes the degradation process in all the compartments. Degradation D-value for each compartment ($D_{\text{degradation}}$) is calculated as follows:

$$D_{\text{degradation}} = k_{reac} V_{bulk} Z_{bulk} \quad \text{(Equation 1)}$$

where

$D_{degredation}$: degradation D-value for each compartment (mol/h/Pa)

k_{reac} : first-order reaction rate constant (h^{-1}) (calculated using the half-life value – **(halflife_ocean, halflife_sediment)**

V_{bulk} : bulk volume of the compartment (m^3)

Z_{bulk} : bulk Z-value for the compartment (mol/ m^3/Pa)

3.2. betr_advective_loss

3.2.1. 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:

$$D_{burial} = AU_{burial} Z_{sbulk} \quad \text{(Equation 2)}$$

D_{burial} : sediment burial D-value for the sediment compartment (mol/h/Pa)

A : Total surface area (m^2) (**A**)

U_{burial} : sediment burial rate (m/h) (**sedburial**)

Z_{sbulk} : bulk Z-value for the sediment compartment (mol/m^3/Pa)

3.2.2. 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:

$$D_{adv} = GZ_{wbulk} \quad \text{(Equation 3)}$$

where

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

G : water outflow rate from the ocean compartment (m^3/h) (**G**)

Z_{wbulk} : bulk Z-value for the ocean compartment (mol/m^3/Pa)

3.3. 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:

$$D_{diffloss} = A\frac{1}{(\frac{1}{k_a Z_a} + \frac{1}{k_w Z_w})} \quad \text{(Equation 4)}$$

where

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

A : total surface area (m^2) (**A**)

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

Z_a : 1/(R×T) (R: ideal gas constant (8,314 m^3-Pa/mol-K); T: ambient temperature (K))

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

Z_w : Z-value for the upper ocean water (mol/m^3/Pa)

3.4. 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 ($D_{partsett}$) is calculated as follows:

$$D_{partsett} = AU_{partsett} Z_{ss} \quad \text{(Equation 5)}$$

where

$D_{partsett}$: particle settling D-value for the ocean compartment (mol/h/Pa)

A : Total surface area (m^2) (**A**)

$U_{partsett}$: particle settling rate (m/h) **(partsett)**

Z_{ss} : Z-value for suspended solids (mol/m^3/Pa)

3.5. 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:

$$D_{resusp} = AU_r Z_s \quad \text{(Equation 6)}$$

where

D_{resusp} : sediment resuspension D-value for the ocean compartment (mol/h/Pa)

A : Total surface area (m^2) (**A**)

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

Z_s : Z-value for sediment solids (mol/m^3/Pa)

3.6. 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:

$$D_{deposit} = AU_{dep}Z_{ss} \quad \text{(Equation 7)}$$

where

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

A : Total surface area (m^2) (**A**)

U_{dep} : sediment deposition rate (m/h) **(seddep)**

Z_{ss} : Z-value for suspended solids (mol/m3/Pa)

3.7. 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:

$$D_{diff} = Ak_{w\text{-}s}Z_w \quad \text{(Equation 8)}$$

where

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

A : total surface area (m^2) (**A**)

$k_{w\text{-}s}$: sediment-water diffusion mass transfer coefficient (m/h) **(diff7water)**

Z_w : Z-value for the lower ocean water (mol/m^3/Pa)

4. COMPARTMENT VOLUMES

Module “volumes” in the folder …/PY/ calculates the compartment and sub-compartment volumes (m^3). 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.

4.1. V1 (Upper Ocean Compartment) and V2 (Lower Ocean Compartment)

These two methods describe 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 ($V_{oceanbulk}$) is calculated as follows:

$$V_{oceanbulk} = Af_{Aocean}h \quad \text{(Equation 9)}$$

where

$V_{oceanbulk}$: bulk volume of the ocean compartment (m^3)

A : total surface area (m^2) **(A)**

f_{Aocean} : 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 (V_{sussed}) is calculated as follows:

$$V_{sussed} = V_{oceanbulk} f_p \quad \text{(Equation 10)}$$

where

V_{sussed} : volume of suspended solids in the ocean compartment (m^3)

$V_{oceanbulk}$: bulk volume of the upper ocean compartment (m^3)

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

Volume of water in the ocean compartment (V_{water}) is calculated as follows:

$$V_{water} = V_{oceanbulk} - V_{sussed} \quad \text{(Equation 11)}$$

where

V_{water} : volume of the water in the ocean compartment (m^3)

$V_{oceanbulk}$: bulk volume of the ocean compartment (m^3)

V_{sussed} : volume of suspended solids in the ocean compartment (m^3)

4.2. 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 ($V_{sedbulk}$) is calculated as follows:

$$V_{sedbulk} = A f_{Aocean} h_7 \quad \text{(Equation 12)}$$

where

$V_{sedbulk}$: bulk volume of the sediment compartment (m^3)

A : total surface area (m^2) **(A)**

f_{Aocean} : fraction of surface covered by coastal water **(perc5)**

h_7 : average sediment compartment depth (m) **(h7)**

Volume of water in the sediment compartment (V_{water}) is calculated as follows:

$$V_{water} = V_{sedbulk} f_{sedwater} \quad \text{(Equation 13)}$$

where

V_{water} : volume of water in the sediment compartment (m^3)

$V_{sedbulk}$: bulk volume of the sediment compartment (m^3)

$f_{sedwater}$: volume fraction of pore water in sediment **(fw7)**

Volume of solids in the sediment compartment (V_{solids}) is calculated as follows:

$$V_{solids} = V_{sedbulk} f_{sedsolids} \quad \text{(Equation 14)}$$

V_{solids} : volume of solids in the sediment compartment (m^3)

$V_{sedbulk}$: bulk volume of the sediment compartment (m^3)

$f_{sedsolids}$: volume fraction of solids in sediment **(fs7)**

5. Z-VALUES

Module "zvalues" in the folder …/PY/ calculates the Z-values (mol/m^3Pa) 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.

5.1. Z1 and Z2 (Upper Ocean Compartment and Lower Ocean Compartment)

These methods describe 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 (Z_{water}) is calculated as follows:

$$Z_{oceanwater} = 0.8(RTK_{aw})^{-1} \quad \text{(Equation 15)}$$

where

$Z_{oceanwater}$: Z-value of ocean water (mol/m^3Pa)

R : ideal gas constant (8.314 m^3Pa/molK)

T : temperature of the compartment (K)

K_{aw} : air-water partition coefficient

Z-values for suspended sediment in the ocean compartment (Z_{sussed}) is calculated as follows:

$$Z_{sussed} = Z_{water} K_{qw} \quad \text{(Equation 16)}$$

where

Z_{sussed} : Z-value of suspended sediment in the ocean compartment (mol/m^{3}Pa)

$Z_{oceanwater}$: Z-value of ocean water (mol/m^{3}Pa)

K_{qw} : suspended sediment - water partition coeffcient

Suspended sediment-water partition coeffcient (K_{qw}) is calculated as follows:

$$K_{qw} = \frac{0.41 K_{ow} f_{ocp} \rho_p}{1000} \quad \text{(Equation 17)}$$

where

K_{qw} : suspended sediment - water partitioning coeffcient

0.41 : the factor defining the relationship between K_{ow} and the K_{oc} (L/kg)

K_{ow} : octanol-water partition coefficient

f_{ocp} : mass fraction of organic carbon in particles in ocean water **(focp1 or focp2)**

ρ_p : density of particles in water (kg/m^3) **(rhop45)**

Z-value for the bulk ocean ($Z_{oceanbulk}$) is calculated as follows:

$$Z_{oceanbulk} = (1 - f_p) Z_{water} + f_p Z_{sussed} \quad \text{(Equation 18)}$$

where

$Z_{oceanbulk}$: Z-value of the bulk ocean (mol/m^{3}Pa)

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

$Z_{oceanwater}$: Z-value of ocean water (mol/m^{3}Pa)

Z_{sussed} : Z-value of suspended sediment in the ocean compartment (mol/m^{3}Pa)

Z-value for the air boundary layer over the upper ocean water (Z_{air}) is calculated as follows:

$$Z_{air} = \frac{1}{RT} \quad \text{(Equation 19)}$$

where

Z_{air} : Z-value of air boundary layer over the upper ocean compartment (mol/m^{3}Pa)

R : ideal gas constant (8.314 m^3Pa/molK)

T : temperature of compartment (K)

5.2.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 ($Z_{sedwater}$) is calculated as follows:

$$Z_{sedwater} = (RTK_{aw})^{-1} \quad \text{(Equation 20)}$$

where

$Z_{sedwater}$: Z-value of sediment water (mol/m^3Pa)

R : ideal gas constant (8.314 m^3Pa/molK)

T : temperature of compartment (K)

K_{aw} : air-water partition coefficient

Z-value for solids in the sediment compartment (Z_{solids}) is calculated as follows:

$$Z_{solids} = Z_{sedwater} K_{sedw} \quad \text{(Equation 21)}$$

where

Z_{solids} : Z-value of solids in sediment (mol/m^3Pa)

$Z_{sedwater}$: Z-value of sediment water (mol/m^3Pa)

K_{sedw} : solids in sediment - water partitioning coefficient

Solids in sediment - water partitioning coefficient (K_{sedw}) is calculated as follows:

$$K_{sedw} = \frac{0.41 K_{ow} f_{ocs} \rho_s}{1000} \quad \text{(Equation 22)}$$

where

K_{sedw} : solids in sediment - water partitioning coefficient

0.41 : the factor defining the relationship between K_{ow} and the K_{oc} (L/kg)

K_{ow} : octanol-water partition coefficient

f_{ocs} : mass fraction of organic carbon in solids in sediment **(focs7)**

ρ_s : density of solids in sediment (kg/m^3) **(rhos7)**

Z-value for the bulk sediment ($Z_{sedbulk}$) is calculated as follows:

$$Z_{sedbulk} = f_w Z_{sedwater} + f_s Z_{solids} \quad \text{(Equation 23)}$$

where

$Z_{sedbulk}$: Z-value of the bulk sediment (mol/m^{3}Pa)

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

$Z_{sedwater}$: Z-value of sediment water (mol/m^{3}Pa)

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

Z_{solids} : Z-value of solids in sediment (mol/m^{3}Pa)

6. INSTALLATION

6.1. Installing the Required Software Packages

In order to run BETR-QWASI-LU, a python interpreter and several add-on packages for scientific computing are required. BETR-QWASI-LU code is written in Python version 3 and all the add-on packages should also be compatible with Python 3.

Below is a list of required software packages:

- Python version 3.x
- Numpy (version 1.11.0 or later)
- Scipy (version 0.17.0 or later)
- Matplotlib (for plotting the results)
- Seaborn (for statistical data visualization)

It is possible to install the required software packages manually. However, it is also possible to install the Python 3 version of **Anaconda Python Distribution**, which is an open-source data science platform.

You can click on the links below to see Anaconda installation in different operating systems.

- https://docs.anaconda.com/anaconda/install/windows/
- https://docs.anaconda.com/anaconda/install/mac-os/
- https://docs.anaconda.com/anaconda/install/linux/

When Anaconda is installed, **Python interpreter**, **Numpy**, **Scipy** and **Matplotlib** packages are installed together. Conda tool that comes with the Anaconda installation makes it very easy to install any additional packages.

seaborn can be installed through conda install using the following command in Anaconda prompt:

```
> conda install seaborn
```

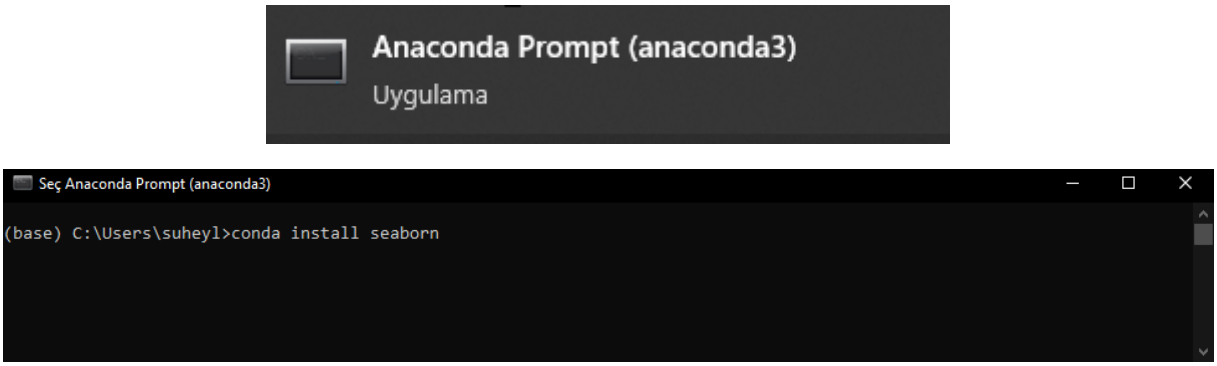

Figure 3. Installing an external Python library using Conda in Anaconda Prompt

6.2. Downloading BETR-QWASI-LU

After installing the required software packages, you can download BETR-QWASI-LU and start running your model simulations:

- Download BETR-QWASI-LU from the project repository on GitHub: https://github.com/rkgoktas/BETR-QWASI-LU-v1.0

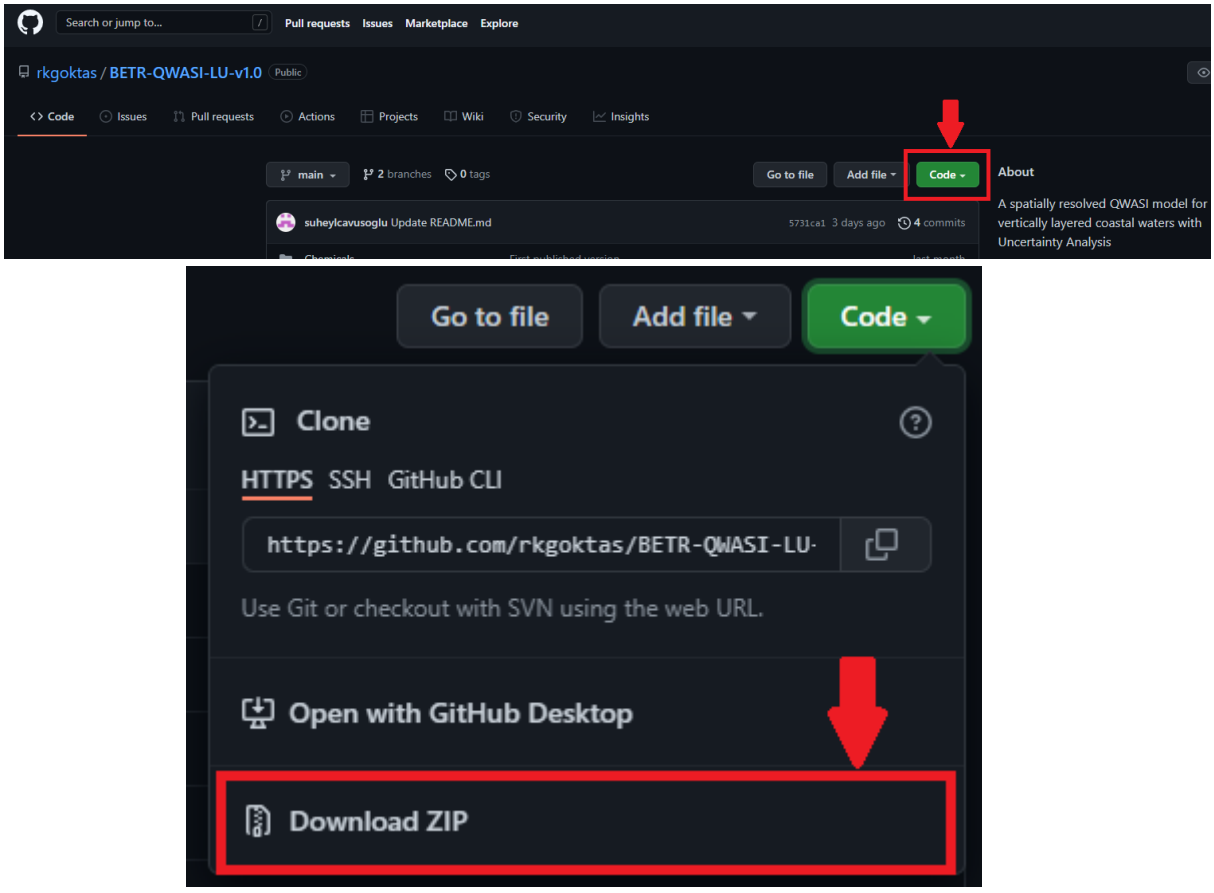

Figure 4. Downloading BETR-QWASI-LU from the project repository on GitHub.

- Unpack BETR-QWASI-LU into an arbitrary directory.
- Go over the tutorials and start experimenting with the provided example run-files.

7. TUTORIALS

Together with the source code of BETR-QWASI-LU, several run-files are also distributed in order to demonstrate how to set-up different types of simulations: (i) steady-state simulations, (ii) dynamic simulations, (iii) Monte Carlo simulations for uncertainty analysis. The example run-files demonstrate the capabilities of BETR-QWASI-LU by conducting multimedia simulations for analyzing the polycyclic aromatic hydrocarbon (PAHs) fate in Izmit Bay, Turkey (Figure 5).

The example run-files provided are Python scripts that work as user interface for the model. The code given in the scripts are extensively commented to facilitate user understanding and customization. The variables that define model inputs in the example run-files can be modified to run model simulations for other chemicals and other environments. The variables that define input files for model runs were explained in section 2. An introductory knowledge of Python will be helpful for the model user.

Three example run-files are included for conducting multimedia simulations for PAH chemicals using BETR-QWASI-LU:

Table 7. Run-files for the tutorials.

run-file	Description of the simulation
runALL_ss_QWASI_2BasinIzmit.py	*Steady-state* simulation for 16 priority PAHs in *Izmit Bay*
runBaP_dyn_QWASI_2BasinIzmit.py	*Dynamic* simulation for Benzo(a)pyrene in *Izmit Bay*
runBaP_ss_U_QWASI_2BasinIzmit.py	*Steady-state* simulation with uncertainty analysis for Benzo(a)pyrene in *Izmit Bay*

Figure 5. Izmit Bay and its two basins modeled as two separate cells.

7.1.1. Steady-state Simulations

The example steady-state run-file "runALL_ss_QWASI_2BasinIzmit.py" can be run to conduct steady-state simulations of the fate of 16 priority PAHs in Izmit Bay using the provided input files. The input parameters listed and explained in Table 8 can be modified in the run-file (Figure 6) for new runs. The example steady-state run-file produces the output files explained in Table 9.

Table 8. Input parameters defined in the run-file for steady-state simulations tutorial (runALL_ss_QWASI_2BasinIzmit.py)

Variable Name	Variable Value	Description
runID	NaP_ss, AcNP_ss, AcN_ss, Flo_ss, PhA_ss, Ant_ss, Flrn_ss, Pir_ss, BaA_ss, Kri_ss, BbF_ss, BkF_ss, BaP_ss, IP_ss, DahA_ss, BghiP_ss	output names
emisfile	Emission_NaP.txt, Emission_AcNP.txt, Emission_AcN.txt, Emission_Flo.txt, Emission_PhA.txt, Emission_Ant.txt, Emission_Flrn.txt, Emission_Pir.txt, Emission_BaA.txt, Emission_Kri.txt, Emission_BbF.txt, Emission_BkF.txt, Emission_BaP.txt, Emission_IP.txt, Emission_DahA.txt, Emission_BghiP.txt	emissions of 16 priority PAHs into the Izmit Bay compartments
seasparfile	seasonal_parameters_QWASI_2BasinIzmit.txt	seasonally varying parameters for Izmit Bay
constparfile	const_parameters_QWASI_2BasinIzmit.txt	seasonally constant parameters for Izmit Bay
flowdirectory	QWASI_2BasinIzmit_Layered	flows between Izmit Bay compartments
chemdata	chemicals_PAH.txt	chemical properties
chemnr	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]	selection of chemicals from chemical properties files
compfile	compartments_QWASI.txt	compartments used in the model
procfile	processes_QWASI.txt	processes used in the model
contfile	control_QWASI.txt	some simulation options
solvfile	solvparams_default.txt	options for the ODE solver

```
runID = ['NaP_ss', 'AcNP_ss', 'AcN_ss', 'Flo_ss', 'PhA_ss', 'Ant_ss', 'Flrn_ss',\
         'Pir_ss', 'BaA_ss', 'Kri_ss', 'BbF_ss', 'BkF_ss','BaP_ss', 'IP_ss',\
         'DahA_ss', 'BghiP_ss'] # output names
years = [list(range(1,5))]*len(runID)    # range of modeling run (years)

#emisdir = ['Emission_BDE209_10_comparts']  # emission inventory ('Emissions/annual/')
emisfile = ['Emission_NaP.txt','Emission_AcNP.txt','Emission_AcN.txt', 'Emission_Flo.txt',\
            'Emission_PhA.txt','Emission_Ant.txt','Emission_Flrn.txt','Emission_Pir.txt',\
            'Emission_BaA.txt','Emission_Kri.txt','Emission_BbF.txt','Emission_BkF.txt',\
            'Emission_BaP.txt','Emission_IP.txt','Emission_DahA.txt','Emission_BghiP.txt'] # emission inventory ('Emissions/')
seasparfile = ['seasonal_parameters_QWASI_2BasinIzmit.txt']*len(runID)#  seasonally varying parameters ('Environment/)
constparfile = ['const_parameters_QWASI_2BasinIzmit.txt']*len(runID)  # seasonally constant parameters ('Environment/')
flowdirectory = ['QWASI_2BasinIzmit_Layered']*len(runID)  # flows in the atmosphere, ocean and fresh water ('Flows/)

chemdata = ['chemicals_PAH.txt']*len(runID)  # chemical properties ('Chemicals/')
chemnr = [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]  # selection of chemical from chemical properties files
compfile = ['compartments_QWASI.txt']*len(runID)   # compartments used in the model ('Environment/')

procfile = ['processes_QWASI.txt']*len(runID)   # processes used in the model  ('Processes/')
contfile = ['control_QWASI.txt']*len(runID)      # some options ('Control/')
solvfile = ['solvparams_default.txt']*len(runID)    # options for ODE solver  ('Solver/')
```

Figure 6. Assignment of input parameters in "runALL_ss_QWASI_2BasinIzmit.py".

Table 9. Output parameters defined in the run-file for steady-state simulations tutorial (runALL_ss_QWASI_2BasinIzmit.py)

Outputs	Description
ss.txt	steady state amounts in all model compartments in mols
summary.txt	summary of model inputs
ss_out.cpk	steady state outputs in specified units as a pickle file
Z_1_air.csv	Z-values for air in compartment 1
[chem]_ss_betr_diff_loss.csv	Diffusive loss rates for chemical [chem]
ssResults.csv	steady state results for all the runs specified in the run-file

7.1.2. Dynamic Simulations

The example run-file "runBaP_dyn_QWASI_2BasinIzmit.py" can be run to conduct dynamic simulations of the fate of benzo[a]pyrene in Izmit Bay using the provided input files. The input parameters listed and explained in Table 10 can be modified in the run-file (Figure 7) for new runs. The example dynamic run-file produces the output files explained in Table 11.

Table 10. Input parameters defined in the run-file for dynamic simulations tutorial (runALL_dyn_QWASI_2BasinIzmit.py)

Variable Name	Variable Value	Description
runID	BaP_dyn_QWASI_2BasinIzmit	output names
years	list(range(1,20))	defines the length of simulation (19 years in this case)
emisfile	Emission_BaP.txt	emissions of BaP into the Izmit Bay compartments
seasparfile	seasonal_parameters_QWASI_2BasinIzmit.txt	seasonally varying parameters for Izmit Bay
constparfile	const_parameters_QWASI_2BasinIzmit.txt	seasonally constant parameters for Izmit Bay
flowdirectory	QWASI_2BasinIzmit_Layered	flows between Izmit Bay compartments
chemdata	chemicals_PAH.txt	chemical properties
chemnr	[13] = BaP	selection of chemical from chemical properties files
compfile	compartments_QWASI.txt	compartments used in the model
procfile	processes_QWASI.txt	processes used in the model
contfile	control_QWASI.txt	some simulation options
solvfile	solvparams_default.txt	options for the ODE solver

```
34  runID = ['BaP_dyn_QWASI_2BasinIzmit'] # output names
35  years = [list(range(1,20))]*len(runID)    # range of modeling run (years)
36
37  #emisdir = ['Emission_BDE209_10_comparts']  # emission inventory ('Emissions/annual/')
38  emisfile = ['Emission_BaP.txt']*len(runID) # emission inventory ('Emissions/')
39  seasparfile = ['seasonal_parameters_QWASI_2BasinIzmit.txt']*len(runID)#  seasonally varying parameters ('Environment/)
40  constparfile = ['const_parameters_QWASI_2BasinIzmit.txt']*len(runID)  # seasonally constant parameters ('Environment/')
41  flowdirectory = ['QWASI_2BasinIzmit_Layered']*len(runID)  # flows in the atmosphere, ocean and fresh water ('Flows/)
42
43  chemdata = ['chemicals_PAH.txt']*len(runID)  # chemical properties ('Chemicals/')
44  chemnr = [13]*len(runID)  # selection of chemical from chemical properties files
45  compfile = ['compartments_QWASI.txt']*len(runID)   # compartments used in the model ('Environment/')
46
47  procfile = ['processes_QWASI.txt']*len(runID)   # processes used in the model  ('Processes/')
48  contfile = ['control_QWASI.txt']*len(runID)      # some options ('Control/')
49  solvfile = ['solvparams_default.txt']*len(runID)    # options for ODE solver  ('Solver/')
```

Figure 7. Assignment of input parameters in “runBaP_dyn_QWASI_2BasinIzmit.py”.

Table 11. Output parameters defined in the run-file for dynamic simulations tutorial (runALL_dyn_QWASI_2BasinIzmit.py)

Outputs	Description
endstate.19.txt	amount of chemical in mols in all the compartments at the end of the simulation
summary.txt	summary of model inputs
Figures UpperOcean.png, Sediment.png, LowerOcean.png, Central_Upper.png, Eastern_Upper.png, Eastern_Lower.png, Central_Lower.png, Eastern_sediment.png, Central_sediment.png	plots of simulated concentrations versus time

7.1.3. Monte Carlo Simulations for Uncertainty Analysis

The example run-file "runBaP_ss_U_QWASI_2BasinIzmit.py" can be run to conduct Monte Carlo simulations for the fate of benzo[a]pyrene in Izmit Bay using the provided input files. The input parameters listed and explained in Table 12 can be modified in the run-file (Figure 8) for new runs. The example Monte Carlo run-file produces the output files explained in Table 13.

Table 12. Input parameters defined in the run-file for uncertainty analysis simulations tutorial (run_ss_U_QWASI_2BasinIzmit.py)

Variable Name	Variable Value	Description
monte_carlo	True	switch on/off Monte Carlo simulations
mc_iter	10000	assign the number of Monte Carlo iterations
runID	BaP_ss_U	output name
emisfile	emission_BaP.txt	emissions of BaP into the Izmit Bay compartments
seasparfile	seasonal_parameters_QWASI_2BasinIzmit.txt	seasonally varying parameters for Izmit Bay
constparfile	const_parameters_QWASI_2BasinIzmit.txt	seasonally constant parameters for Izmit Bay
u_envpar	{'fp1':3, 'fp2':3, 'partsett':3, 'seddep':3, 'focs7':1.5, 'fs7':3, 'rhos7':1.5, 'sedburial':3, 'sedresup':3, 'h7':2, 'tair2':1.1, 'Gup':3, 'Glow':3}	define the uncertain environmental parameters and their k-values
flowdirectory	QWASI_2BasinIzmit_Layered	flows between Izmit Bay compartments
chemdata	chemicals_PAH.txt	chemical properties
chemnr	[13] = BaP	selection of chemical from chemical properties files
u_chempar	{'logKaw':1.5, 'logKow':1.1, 'halflife_sediment':3}	define the uncertain chemical parameters and their k-values
compfile	compartments_QWASI.txt	compartments used in the model
procfile	processes_QWASI.txt	processes used in the model
contfile	control_QWASI.txt	some simulation options
solvfile	solvparams_default.txt	options for the ODE solver

```
monte_carlo = True # SWITCH ON/OFF MONTE CARLO SIMULATIONS, RKG, 20.01.2022
mc_iter = 10000    # assign the number of Monte Carlo iterations, RKG, 20.01.2022
use_odespy = False       #SWITCH ON/OFF FAST SOLVER
track_fluxes = False    #SWITCH ON/OFF FLUX INTEGRATION
track_se = False         #SWICH ON/OFF TRACKING OF SECONDARY EMISSIONS
use_correction = False   #SWICH ON/OFF flow with correction

## options
"""
Change to current Directory to ensure that relative paths are set correctly

Tends to cause problem under Windows otherwise

"""

abspath=os.path.abspath(__file__)
dname = os.path.dirname(abspath)
os.chdir(dname)

runID = ['BaP_ss_U'] # output names
years = [list(range(1,5))]*len(runID)    # range of modeling run (years)

#emisdir = ['Emission_BDE209_10_comparts']  # emission inventory ('Emissions/annual/')
emisfile = ['emission_BaP.txt']*len(runID) # emission inventory ('Emissions/')
seasparfile = ['seasonal_parameters_QWASI_2BasinIzmit.txt']*len(runID)#  seasonally varying parameters ('Environment/)
constparfile = ['const_parameters_QWASI_2BasinIzmit.txt']*len(runID)  # seasonally constant parameters ('Environment/')
u_envpar = {'fp1':3, 'fp2':3, 'partsett':3, 'seddep':3, 'focs7':1.5, 'fs7':3,\
            'rhos7':1.5, 'sedburial':3, 'sedresup':3, 'h7':2, 'tair2':1.1,\
            'Gup':3, 'Glow':3} # define the uncertain environmental parameters and their k-values
flowdirectory = ['QWASI_2BasinIzmit_Layered']*len(runID)  # flows in the atmosphere, ocean and fresh water ('Flows/)

chemdata = ['chemicals_PAH.txt']*len(runID)  # chemical properties ('Chemicals/')
chemnr = [13]*len(runID)  # selection of chemical from chemical properties files
u_chempar = {'logKaw':1.5, 'logKow':1.1, 'halflife_sediment':3} # define the uncertain chemical parameters and their k-values
compfile = ['compartments_QWASI.txt']*len(runID)   # compartments used in the model ('Environment/')

procfile = ['processes_QWASI.txt']*len(runID)   # processes used in the model  ('Processes/')
contfile = ['control_QWASI.txt']*len(runID)      # some options ('Control/')
solvfile = ['solvparams_default.txt']*len(runID)    # options for ODE solver  ('Solver/')
```

Figure 8. Assignment of input parameters in “runBaP_ss_U_QWASI_2BasinIzmit.py”.

Table 13. Output parameters defined in the run-file for uncertainty analysis simulations tutorial (run_ss_U_QWASI_2BasinIzmit.py)

Outputs	Description
mc.txt	Monte Carlo simulation inputs and outputs
summary.txt	summary of model inputs
ss_out.cpk	steady state outputs in specified units as a pickle file
mc_cell_1.xlsx	inputs and outputs of each Monte Carlo iteration in cell 1
mc_cell_0.xlsx	inputs and outputs of each Monte Carlo iteration in cell 1
Figures sr2_merkez.png, sr2_doğu.png	heat maps of squared Spearman rank correlation coefficients