# Package 'isobxr'

July 23, 2021

| Type Package   |                                   |
|--|-----------------------------------|
| Title Stable isotope box modelling in R  |                                   |
| Version 0.1.0  |                                   |
| <b>Description</b> A set of functions to run simple and composite box-models to describe the dynamic or static distribution of stable isotopes in open or closed systems. The package also allows the sweeping of many parameters in both static and dynamic conditions. It also comes with a post-run plotting interface built under shiny. |                                   |
| <b>Depends</b> R (>= 3.5.0)  |                                   |
| License GPL-3  |                                   |
| <pre>URL https://github.com/ttacail/isobxr</pre>   |                                   |
| <pre>BugReports https://github.com/ttacail/isobxr/issues</pre>   |                                   |
| Encoding UTF-8   |                                   |
| LazyData false   |                                   |
| Imports stringr, readxl, dplyr, data.table, deSolve, rlang, grid, metR, shiny, shinyFiles, shinythemes, shinyjs, DT, ggplot2, ggrepel, qgraph, writexl   |                                   |
| RoxygenNote 7.1.1  |                                   |
| Suggests knitr, rmarkdown, devtools  |                                   |
| VignetteBuilder knitr  |                                   |
| R topics documented:   |                                   |
| 1 – 7  | 2<br>3<br>5<br>6<br>6<br>11<br>12 |
| Index  | 15                                |

2 ana\_slvr

| ana_slvr | Analytically solve stable isotope box models |
|----------|--|
|          |  |

## **Description**

An analytical solver of the system of ordinary differential equations (ODES) of stable isotope ratios of element X in all boxes.

Not intended for direct use although possible.

The analytical solver finds the eigenvalues and eigenvectors of the ODES.

Given the initial conditions as specified in IN.Rda file, it determines the set of analytical solutions that describes the evolution of isotope ratios in each box over time.

# Usage

```
ana_slvr(input_path, to_DIGEST_csv = FALSE)
```

## Arguments

input\_path path to the INPUT file containing all commands for the run (character string, file name structure: *RUN name* + \_*IN.Rda*)

to\_DIGEST\_csv edit csv outputs or not (logical) to the RUN DIGEST folder (logical, default is FALSE)

### Value

The function returns the analytically determined evolution of stable isotope compositions in all boxes over the run duration as specified in INPUT file.

The outputs of the run are stored in a Rda output file with the following file name structure:  $RUN\ name + \_OUT.Rda$ 

## Optional csv outputs to the DIGEST folder are as follows

- 1. OUT data file with initial and final size and delta values in all boxes. (file name structure: *out\_1\_A\_OUT + RUN name + .csv*)
- 2. ODE\_SOLNs data file summarizing outputs of the analytical solutions of the ODES (eigenvalues, eigenvectors, relaxation times, constants according to initial conditions). (file name structure: out\_2\_A\_ODE\_SOLNs + RUN name + .csv)
- 3. evD data file of the evolution with time of the delta values in all boxes. (file name structure: *out\_3\_A\_evD + RUN name + .csv*)

compose\_isobxr 3

compose\_isobxr

Compose a stable isotope box model scenario

## **Description**

A function to compose an isobxr box model scenario, defined by a series of n successive runs, each run inheriting from the final state conditions of the previous run.

It is possible to force parameters at each run, namely:

#### 1. fluxes

(overwriting all or a subset of fluxes defined in O\_ISOBXR\_MASTER.xlsx master file)

2. isotope fractionation coefficients

(overwriting all or a subset of coefficients defined in *O\_ISOBXR\_MASTER.xlsx* master file)

3. box sizes

(overwriting all or a subset of box sizes defined in *0\_ISOBXR\_MASTER.xlsx* master file)

- 4. rayleigh isotope distillation
- 5. isotope composition of a source box at initial state

## Usage

```
compose_isobxr(
  workdir,
  SERIES_ID,
  time_units,
  COMPO_MASTER,
  plot_HIDE_BOXES_delta = NULL,
  plot_HIDE_BOXES_size = NULL,
  EACH_RUN_DIGEST = FALSE,
  to_CPS_DIGEST_CSVs = FALSE
)
```

## **Arguments**

workdir

Working directory of **0\_ISOBXR\_MASTER.xlsx** master file, of the composite master file (e.g., **0\_COMPO\_MASTER.xlsx**) and where output files will be stored. (character string)

(character stri

SERIES\_ID

Name of the composite model series the run belongs to.

It determines the folder in which the output files will be stored for this composite

un.

A composite run number is automatically linked to it, subsequent runs can not overwrite a previous composite run.

(character string)

time\_units

Vector defining the initial time unit (identical to unit used in fluxes), followed by the time unit used for the graphical output.

Character string, to be selected amongst the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* e.g., c("d", "yr") to convert days into years

4 compose\_isobxr

COMPO\_MASTER

Name of the composite master file (e.g.,  $\theta$ \_COMPO\_MASTER.xlsx), defining the composite run scenario.

(character string)

plot\_HIDE\_BOXES\_delta

**OPTIONAL** 

Vector of character strings,

defining the names of the boxes to hide in the plot of the delta values as a function of time, edited as a pdf.

 $(e.g.,\,c("BOX\_A",\,"BOX\_C"))$ 

Default is NULL (no box hidden).

plot\_HIDE\_BOXES\_size

**OPTIONAL** 

Vector of character strings,

defining the names of the boxes to hide in the plot of the box sizes (masses of X) as a function of time, edited as a pdf.

(e.g., c("BOX\_A", "BOX\_C"))

Default is NULL (no box hidden).

EACH\_RUN\_DIGEST

OPTIONAL

Logical value.

Edits full digests for each model run (all optional outputs of run\_isobxr function) if TRUE.

Default is FALSE.

to\_CPS\_DIGEST\_CSVs

**OPTIONAL** 

Logical value.

Exports all global csv outputs to  $\theta$ \_*CPS\_DIGEST* folder (full evD and full evS) if TRUE.

Default is FALSE.

#### Value

Creates and stores all outputs in a dedicated composite SERIES directory located in working directory, with the following name structure:

**3\_CPS + SERIES\_ID + YYY**, where YYY is a composite scenario number automically set between 001 and 999.

No overwriting of previous composite runs is possible.

1. Creates the set of inputs and outputs for all successive *n* runs,

numbered from to 1 to *n* in an XXXX format with the following format:

 $CPS + SERIES\_ID + YYY + XXXX + IN.Rda$ 

 $CPS + SERIES\_ID + YYY + XXXX + OUT.Rda$ 

(see run\_isobxr documentation)

- 2. Writes summarized results in the  $\theta$ \_CPS\_DIGEST folder:
  - (a) LOG file of local composite run.

(file name structure: *CPS* + *SERIES\_ID* + *YYY* + *\_LOG.csv*)

(b) Composite master file.

(file name structure: *CPS* + *SERIES\_ID* + *YYY* + *\_MASTER.xlsx*)

(c) Dataset of temporal evolution of delta values (evD) in all boxes over the n runs that constitute the composite run scenario

(file name structure: *CPS* + *SERIES\_ID* + *YYY* + *evD.RDS*)

num\_slvr 5

(d) Dataset of temporal evolution of box sizes (evS, masses of X) in all boxes over the *n* runs that constitute the composite run scenario

(file name structure: *CPS* + *SERIES\_ID* + *YYY* + *evS.RDS*)

- (e) All-in-one plot of the evolution of delta values + sizes in all non hidden boxes. (file name structure:  $CPS + SERIES\_ID + YYY + p\_evDS.pdf$ )
- (f) Multiple plots of the evolution of delta values in all non hidden boxes. (file name structure: *CPS* + *SERIES\_ID* + *YYY* + *pf\_evD.pdf*)
- (g) Multiple plots of the evolution of box sizes in all non hidden boxes. (file name structure: *CPS* + *SERIES\_ID* + *YYY* + *pf\_evS.pdf*)

## **Optional outputs**

1. If EACH\_RUN\_DIGEST = TRUE

Creates and fills **DIGEST** folder for each run of the composite scenario with all optional outputs of run\_isobxr function.

(folder name structure: *CPS* + *SERIES\_ID* + *YYY* + *XXXX* + *DIGEST*)

2. If to\_CPS\_DIGEST\_CSVs = TRUE

In the  $\theta$ \_CPS\_DIGEST folder, edits csv versions of the whole-composite scenario evD and evS datasets.

(file names structures:  $CPS + SERIES\_ID + YYY + evD.csv$  and  $CPS + SERIES\_ID + YYY + evS.csv$ )

#### See Also

Documentation on run\_isobxr

num\_slvr

Numerically solve stable isotope box models

## **Description**

A numerical solver of the system of ordinary differential equations (ODES), describing the evolution of stable isotope ratios in all boxes of a system.

Not intended for direct use although possible.

The numerical solver uses the ode function of the deSolve package to integrate the stable isotopes ratios over time in each box. It allows the calculation of the evolution of stable isotope ratio even in the case of unbalanced outward and inward fluxes of element X in a given box resulting in the accumulation or loss of element X.

#### Usage

```
num_slvr(input_path, to_DIGEST_csv = FALSE)
```

## Arguments

input\_path path to the INPUT file containing all commands for the run

(character string, file name structure: **RUN name + \_IN.Rda**)

(logical, default is FALSE)

#### Value

The function returns the numerically determined evolution of stable isotope compositions and mass of element X in all boxes over the run duration as specified in INPUT file.

The outputs of the run are stored in a Rda output file with the following file name structure:  $RUN\ name + \_OUT.Rda$ 

## Optional csv outputs to the DIGEST folder are as follows

- 1. OUT data file storing initial and final size and delta values in all boxes. (file name structure: *out\_1\_N\_OUT + RUN name + .csv*)
- 2. evS data file storing the evolution with time of the sizes (masses of element X) of all boxes. (file name structure:  $out_2 N_e vS + RUN name + .csv$ )
- 3. evD data file storing the evolution with time of the delta values in all boxes. (file name structure: out\_3\_N\_evD + RUN name + .csv)

runShinyPlots

Call isobxr plot shiny app

## **Description**

A function to call the isobxr plot shiny app to interactively plot outputs from compose\_isobxr, sweep\_steady and sweep\_dyn.

The function takes no arguments but requires the definition of a working directory where all SERIES directory are stored.

This working directory needs to be defined as a character string and stored in a variable called workdir. For instance:

workdir = "User/isobxr\_working\_directory"

## Usage

runShinyPlots()

run\_isobxr

Run isobxr stable isotope box model

# Description

A function to run the isobxr stable isotope box model, assessing the design of the model and automatically running num\_slvr or ana\_slvr depending on the conditions.

#### Usage

```
run_isobxr(
 workdir,
 SERIES_ID,
  flux_list_name,
  coeff_list_name,
  t_lim,
 nb_steps,
  time_units,
 FORCING_RAYLEIGH = NULL,
 FORCING_SIZE = NULL,
 FORCING_DELTA = NULL,
 FORCING_ALPHA = NULL,
 COMPOSITE = FALSE,
 COMPO\_SERIES\_n = NaN,
 COMPO_SERIES_FAMILY = NaN,
 EXPLORER = FALSE,
 EXPLO_SERIES_n = NaN,
  EXPLO_SERIES_FAMILY = NaN,
 HIDE_PRINTS = FALSE,
  to_DIGEST_DIAGRAMS = TRUE,
  to_DIGEST_evD_PLOT = TRUE,
  to_DIGEST_CSV_XLS = FALSE,
 evD_PLOT_time_as_log = TRUE
)
```

# Arguments

workdir Working directory of *0\_ISOBXR\_MASTER.xlsx* master file

and where output files will be stored.

(character string)

SERIES\_ID Name of the model series the run belongs to.

It determines the folder in which the output files will be stored.

(character string)

flux\_list\_name Name of the list of fluxes and initial box sizes to be used for the run,

calling (by its header name) a single column of the FLUXES sheet of the

0 ISOBXR MASTER.xlsx file.

(character string)

coeff\_list\_name

Name of the list of fractionation coefficients to be used for the run,

calling (by its header name) a single column of the COEFFS sheet of the

0\_ISOBXR\_MASTER.xlsx file.

(character string)

t\_lim Run duration, given in the same time units as the fluxes.

(integer)

nb\_steps Number of calculation steps.

It determines the resolution of the run.

(integer)

time\_units Vector defining the initial time unit (identical to unit used in fluxes),

followed by the time unit used for the graphical output.

Character string, to be selected amongst the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* e.g., c("d", "yr") to convert days into years

#### FORCING\_RAYLEIGH

#### **OPTIONAL**

Dataframe describing the forcing on a fractionation coefficient by a Rayleigh isotope distillation,

as a function of flux intensities and a fundamental fractionation coefficient.

Dataframe formatting details are in isobxr vignette.

Default is NULL.

## FORCING\_SIZE OPTIONAL

Dataframe describing the forcing on one or several box sizes (mass of element X).

The newly defined sizes for the given set of boxes overwrite their sizes as previously defined in *0 ISOBXR MASTER.xlsx* file.

Dataframe formatting details are in isobxr vignette.

Default is NULL.

## FORCING\_DELTA OPTIONAL

Dataframe describing the forcing on one or several boxes initial isotope composition expressed as delta values.

The newly defined delta values for the given set of boxes overwrite the delta values as previously defined in *0\_ISOBXR\_MASTER.xlsx* file.

Dataframe formatting details are in isobxr vignette.

Default is NULL.

## FORCING\_ALPHA OPTIONAL

Dataframe describing the forcing on one or several fractionation coefficients from one reservoir to another.

The newly defined alpha values for the given set of boxes overwrite the alpha values as previously defined in *0\_ISOBXR\_MASTER.xlsx* file.

Dataframe formatting details are in isobxr vignette.

Default is NULL.

## COMPOSITE NOT TO BE USED IN SINGLE RUN

Logical value automatically defined in compose\_isobxr.

Default is FALSE.

# COMPO\_SERIES\_n NOT TO BE USED IN SINGLE RUN

Iteration of the composite run for the given series it belongs to, automatically defined in compose\_isobxr.

Default is NaN.

# COMPO\_SERIES\_FAMILY

## NOT TO BE USED IN SINGLE RUN

Composite run series family, automatically defined in compose\_isobxr.

Default is NaN.

## EXPLORER NOT TO BE USED IN SINGLE RUN

Logical value automatically defined in sweep\_steady or sweep\_dyn.

Default is FALSE.

## EXPLO\_SERIES\_n NOT TO BE USED IN SINGLE RUN

Iteration of the sweep run for the given series it belongs to, automatically defined in sweep\_steady or sweep\_dyn.

Default is NaN.

## EXPLO\_SERIES\_FAMILY

NOT TO BE USED IN SINGLE RUN

Sweep run series family, automatically defined in sweep\_steady or sweep\_dyn.

Default is NaN.

## HIDE\_PRINTS OPTIONAL

Logical value.

Prints outputs details in R console if TRUE.

This parameter does not hide the warnings regarding the automatic update of the run duration in case of the emptying of a box.

Default is FALSE.

## to\_DIGEST\_DIAGRAMS

**OPTIONAL** 

Logical value.

Edits pdf of box model diagram in RUN DIGEST folder if TRUE.

Default is TRUE.

#### to\_DIGEST\_evD\_PLOT

**OPTIONAL** 

Logical value.

Edits pdf of delta time evolution plot in RUN DIGEST folder if TRUE.

Default is TRUE.

## to\_DIGEST\_CSV\_XLS

**OPTIONAL** 

Logical value.

Edits xlsx version of the Rda input file (ending with \_IN.xlsx) and all ana\_slvr or num\_slvr CSV output files in RUN DIGEST folder if TRUE.

Default is FALSE.

## evD\_PLOT\_time\_as\_log

**OPTIONAL** 

Logical value.

Print evD plot with log10 time scale as x-axis.

Default is TRUE.

#### Value

If the function is run independently and if directory is not yet existing,

run\_isobxr creates and stores all outputs in a *SERIES* folder located in working directory, with the following name structure:

## $2_RUN + SERIES_ID$

 $1. \ \ Automatically \ sets \ a \ XXXX \ run \ number \ between \ 0001 \ and \ 9999.$ 

The outputs do not overwrite possible identical previously performed runs.

2. Stores all run commands in a file with the Rda format.

This file stores all commands used as arguments for solver function (ana\_slvr or num\_slvr). (file name structure:  $SERIES\_ID + XXXX + \_IN.Rda$ )

This encompasses the following:

- (a) **CONSTS\_IN**: Dataframe documenting the constants (Element, isotopes, reference ratio)
- (b) **INITIAL\_IN**: Dataframe documenting the initial conditions of all box sizes (incl. empty boxes)

and all initial delta values.

(c) **FLUXES\_IN**: Dataframe documenting the massic fluxes of element X between all boxes (structured as a square matrix)

(d) **COEFFS\_IN**: Dataframe documenting the isotopic fractionation coefficients between all boxes (structured as a square matrix)

(e) **BOX\_META\_IN**: Dataframe documenting box metadata

(Box names, initial X masses and delta values, total inward and outward X fluxes in each box.

flux balance for each box, X residence time in each box, max run time before total emptying of each box,

box infinite/finite status, system diagram coordinates)

3. Stores all outputs in a file with the Rda format.

This file stores all data produced by the function.

(file name structure: **SERIES\_ID** + **XXXX** + **\_OUT.Rda**)

4. Updates the general log file, located in general working directory. (file name: *1\_LOG.csv*)

## Optional outputs, stored in DIGEST folder

A *DIGEST* folder is created to store all optional outputs of the run\_isobxr function. The *DIGEST* folder is created in the *SERIES* folder with the following name structure: 2\_RUN + SERIES\_ID / SERIES\_ID + XXXX + DIGEST

 If to\_DIGEST\_CSV\_XLS = TRUE, creates an INPUT file in the xlsx format stored in *DIGEST* folder, containing all run conditions and parameters. (file name structure: *in\_0\_INPUTS* + *SERIES\_ID* + *XXXX* + .*xlsx*)

 If to\_DIGEST\_CSV\_XLS = TRUE, stores csv versions of the num\_slvr or ana\_slvr outputs in *DIGEST* folder. See num\_slvr or ana\_slvr documentation for further details.

3. If to DIGEST DIAGRAMS = TRUE,

edits a Box model diagram of flux (DIAG\_FLUX pdf) of element X (mass per time unit) between all boxes.

(file name structure: *in\_1\_DIAG\_FLUX* + *SERIES\_ID* + *XXXX* + .*pdf*)

4. If to DIGEST DIAGRAMS = TRUE,

edits a Box model diagram of isotope fractionation coefficients (DIAG\_COEFF pdf) between all boxes.

(file name structure:  $in_2\_DIAG\_COEFF + SERIES\_ID + XXXX + .pdf$ )

5. If to\_DIGEST\_evD\_PLOT = TRUE,

edits a pdf plot of the time dependent evolution of delta values together with the evolution of the box sizes (masses of element X).

The time x-axis is a logarithmic scale by default but can be set to linear scale with the evD\_PLOT\_time\_as\_log parameter, if set to FALSE. (file name structure:  $out_0$ \_PLOT\_evD +  $SERIES_ID + XXXX + .pdf$ )

# See Also

Documentation on num\_slvr or ana\_slvr functions.

sweep\_dyn 11

sweep\_dyn

Sweep the space of two parameters during a dynamic run

# Description

A function to assess the influence of two parameters (varying over a range of values) on dynamic evolution of a given model in response to a given perturbation.

# Usage

```
sweep_dyn(
  workdir,
  SERIES_ID,
  time_units,
  EXPLO_MASTER,
  EXPLO_AXIS_1,
  EXPLO_AXIS_2,
  to_DYN_DIGEST_CSVs = FALSE
)
```

## **Arguments**

workdir Working directory of *0\_ISOBXR\_MASTER.xlsx* master file,

of the dynamic sweep master file (e.g.,  $\theta$ \_EXPLO\_DYN\_MASTER.xlsx)

and where output files will be stored.

(character string)

SERIES\_ID Name of the sweep series the run belongs to.

It determines the folder in which the output files will be stored for this sweep

run.

A sweep run number is automatically linked to it, and subsequent sweep runs

can not overwrite a previous one.

(character string)

time\_units Vector defining the initial time unit (identical to unit used in fluxes),

followed by the time unit used for the graphical output. Character string, to be selected amongst the following: micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr

e.g., c("d", "yr") to convert days into years

EXPLO\_MASTER Name of the dynamic sweep master file (e.g., 0\_EXPLO\_DYN\_MASTER.xlsx),

defining the dynamic sweep run scenario.

(character string)

EXPLO\_AXIS\_1 Set of values of sweeping parameter 1.

See Vignette for further details.

EXPLO\_AXIS\_2 Set of values of sweeping parameter 2.

See Vignette for further details.

to\_DYN\_DIGEST\_CSVs

**OPTIONAL** 

Logical value.

Exports all global csv outputs to  $0\_DYN\_DIGEST$  folder (full evD and evS) if TRUE.

Default is FALSE.

12 sweep\_steady

### Value

Creates and stores all outputs in a dedicated dynamic steady SERIES directory located in working directory, with the following name structure:

**4\_DYN** + **SERIES\_ID** + **YYY**, where YYY is a sweep dynamic run number automically set between 001 and 999.

No overwriting of previous sweep dynamic run runs is possible.

- 1. Calculates the number of single runs the sweeping will require depending on the sweeped parameters.
- 2. Asks the user confirmation to run sweep\_dyn, as the run calculation time depends on the number of successive sweeping runs.
- 3. Writes the set of inputs and outputs for all successive *n* sweeping runs, numbered from to 1 to *n* in an XXXX format, with the following name formats:

```
DYN + SERIES_ID + YYY + XXXX + IN.Rda
DYN + SERIES_ID + YYY + XXXX + OUT.Rda
(see run_isobxr documentation).
```

- 4. Writes summarized results in the **0\_DYN\_DIGEST** folder:
  - (a) Archived LOG file of local sweep dynamic run. (file name structure: *DYN* + *SERIES ID* + *YYY* + *LOG.csv*)
  - (b) Archived sweep dynamic master file.
    (file name structure: *DYN* + *SERIES\_ID* + *YYY* + *\_MASTER.xlsx*)
  - (c) Dataset of temporal evolution of delta values (evD) in all boxes over the n runs that constitute the sweep dynamic run.
    - (file name structure:  $DYN + SERIES\_ID + YYY + evD.RDS$ )
  - (d) Dataset of temporal evolution of box sizes (evS, masses of X) in all boxes over the n runs that constitute the sweep dynamic run.

(file name structure: *DYN* + *SERIES\_ID* + *YYY* + *evS.RDS*)

# **Optional output**

1. If to\_DYN\_DIGEST\_CSVs = TRUE

In the **0\_DYN\_DIGEST** folder, edits csv versions of the sweep dynamic run datasets (full evD and evS) with the following name structures:

- (a)  $DYN + SERIES\_ID + YYY + evD.csv$
- (b)  $DYN + SERIES\_ID + YYY + evS.csv$

sweep\_steady

Sweep the space of two parameters at the final state of a run

# **Description**

A function to assess the influence of two parameters (varying over a range of values) on the final state of a given model.

sweep\_steady 13

#### Usage

```
sweep_steady(
  workdir,
  SERIES_ID,
  time_units,
  EXPLO_MASTER,
  EXPLO_AXIS_1,
  EXPLO_AXIS_2,
  to_STD_DIGEST_CSVs = FALSE
)
```

## **Arguments**

workdir Working directory of *0\_ISOBXR\_MASTER.xlsx* master file,

of the steady sweep master file (e.g., 0\_EXPLO\_STEADY\_MASTER.xlsx)

and where output files will be stored.

(character string)

SERIES\_ID Name of the sweep series the run belongs to.

It determines the folder in which the output files will be stored for this sweep

run.

A sweep run number is automatically linked to it, and subsequent sweep runs

can not overwrite a previous one.

(character string)

time\_units Vector defining the initial time unit (identical to unit used in fluxes),

followed by the time unit used for the graphical output. Character string, to be selected amongst the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* 

e.g., c("d", "yr") to convert days into years

EXPLO\_MASTER Name of the steady sweep master file (e.g., *0\_EXPLO\_STEADY\_MASTER.xlsx*),

defining the steady sweep run scenario.

(character string)

EXPLO\_AXIS\_1 Set of values of sweeping parameter 1.

See Vignette for further details.

EXPLO\_AXIS\_2 Set of values of sweeping parameter 2.

See Vignette for further details.

to\_STD\_DIGEST\_CSVs

OPTIONAL

Logical value.

Exports all global csv outputs to **0\_STD\_DIGEST** folder (full and final evD and

evS) if TRUE.

Default is FALSE.

# Value

Creates and stores all outputs in a dedicated sweep steady SERIES directory located in working directory, with the following name structure:

**4\_STD + SERIES\_ID + YYY**, where YYY is a sweep steady run number automically set between 001 and 999.

No overwriting of previous sweep steady run runs is possible.

1. Calculates the number of single runs the sweeping will require depending on the sweeped parameters.

14 sweep\_steady

2. Asks the user confirmation to run sweep\_steady, as the run calculation time depends on the number of successive sweeping runs.

3. Writes the set of inputs and outputs for the single initial run only with the following format:

```
STD + SERIES_ID + YYY + 0001 + IN.Rda
STD + SERIES_ID + YYY + 0001 + OUT.Rda
(see run_isobxr documentation).
```

- 4. Writes summarized results in the *0\_STD\_DIGEST* folder:
  - (a) Archived LOG file of local sweep steady run. (file name structure: *STD* + *SERIES\_ID* + *YYY* + *\_LOG.csv*)
  - (b) Archived sweep steady master file.
    (file name structure: *STD* + *SERIES\_ID* + *YYY* + *\_MASTER.xlsx*)
  - (c) Dataset of temporal evolution of delta values (evD) in all boxes over the n runs that constitute the sweep steady run.

(file name structure: *STD* + *SERIES\_ID* + *YYY* + *evD.RDS*)

- (d) Dataset of temporal evolution of box sizes (evS, masses of X) in all boxes over the n runs that constitute the sweep steady run.
  - (file name structure: *STD* + *SERIES\_ID* + *YYY* + *evS.RDS*)
- (e) Dataset of final state of delta values (evD) in all boxes over the n runs that constitute the sweep steady run.
  - (file name structure: *STD* + *SERIES\_ID* + *YYY* + *evD\_final.RDS*)
- (f) Dataset of final state of box sizes (evS, masses of X) in all boxes over the n runs that constitute the sweep steady run.

(file name structure: *STD* + *SERIES\_ID* + *YYY* + *evS\_final.RDS*)

## **Optional output**

1. If to\_STD\_DIGEST\_CSVs = TRUE

In the  $\theta\_STD\_DIGEST$  folder, edits csv versions of the sweep steady run datasets (full and final evD and evS) with the following name structures:

- (a)  $STD + SERIES\_ID + YYY + evD.csv$
- (b)  $STD + SERIES\_ID + YYY + evS.csv$
- (c) STD + SERIES\_ID + YYY + evD\_final.csv
- (d)  $STD + SERIES\_ID + YYY + evS\_final.csv$

# **Index**

```
ana_slvr, 2, 6, 9, 10

compose_isobxr, 3, 6, 8

num_slvr, 5, 6, 9, 10

run_isobxr, 4, 5, 6, 9, 10, 12, 14

runShinyPlots, 6

sweep_dyn, 6, 8, 9, 11, 12

sweep_steady, 6, 8, 9, 12, 14
```