Package 'isobxr'

August 30, 2021

Type Package

Title Stable Isotope Box Modelling in R

Version 1.0.0

Description 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. The formalisms used in these models are derived from Albarede, 1995, Introduction to Geochemical Modelling, Cambridge University Press, Cambridge <doi:10.1017/CBO9780511622960>.

Depends R (>= 3.5.0)

License GPL-3

URL https://github.com/ttacail/isobxr, https://ttacail.github.io/isobxr_web/, https://ttacail.github.io/isobxr/

BugReports https://github.com/ttacail/isobxr/issues

Encoding UTF-8

LazyData false

Imports stringr, readxl, dplyr, data.table, deSolve, rlang, grid, metR, shiny, shinyFiles, shinythemes, shinyjs, DT, ggplot2, ggrepel, qgraph, writexl, R.utils, fs

RoxygenNote 7.1.1

Suggests knitr, rmarkdown, devtools

VignetteBuilder knitr

R topics documented:

`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, save_run_outputs = 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)
`save_run_outputs`	*OPTIONAL* Logical value. Allows saving all run outputs to directory containing INPUT file. By default, run outputs are stored in a temporary directory and are erased if not exported. 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.

By default (unless save_run_outputs = TRUE), run outputs are stored in the temporary directory and are not exported.

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` *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 *0_ISOBXR_MASTER.xlsx* master file)
2. **isotope fractionation coefficients**
   (overwriting all or a subset of coefficients defined in *0_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,
  plot_results = TRUE,
  save_run_outputs = 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 if exported by user. (character string)
`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 run. 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 among the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* e.g., c("d", "yr") to convert days into years

`COMPO_MASTER` Name of the composite master file (e.g., ***0_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 ***0_CPS_DIGEST*** folder (full evD and full evS) if TRUE.
Default is FALSE.

`plot_results` *OPTIONAL*
Logical value.
If TRUE, plots in R session the composite model run evolution of delta values and box sizes for boxes of interest (see plot_HIDE_BOXES_delta and plot_HIDE_BOXES_size parameters to remove boxes from plots).
Default is TRUE.

`save_run_outputs`
OPTIONAL
Logical value.
Allows saving all run outputs to working directory (workdir).
By default, run outputs are stored in the temporary directory and are erased if not exported.
Default is FALSE.

Value

Calculates the time evolution of delta values and box sizes in all boxes throughout scenario.

`compose_isobxr` returns by default a plot showing time evolution of delta values and box sizes for all boxes
(set plot_deltas = FALSE to mute the plots)

The graphical results of the composite run can be also interactively explored using the `shinobxr_app` function in case user saves the outputs to the working directory (save_run_outputs = TRUE).

compose_isobxr creates a series of isotope data and metadata, all of which are stored in a temporary directory.
The user can save all outputs described below to their working directory by setting save_run_outputs = TRUE (default is FALSE).

compose_isobxr creates and stores all outputs in a dedicated dynamic steady SERIES directory with the following name structure:
3_CPS + SERIES_ID + YYY, where YYY is a composite scenario number automatically set between 001 and 999.
No overwriting of previous composite runs is possible.

compose_isobxr base workflow:

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 ***0_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***)
   (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 ***0_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

Examples

```
# Example 1: Changing intensity of fluxes
# for more information see tutorial at
# https://ttacail.github.io/isobxr_web/vgn_06_compose_isobxr_tutorial.html#34_Run_outputs

# This is an example using the tutorial files embedded in package data
# It can be run as such.
compose_isobxr(workdir = "/Users/username/Documents/1_ABC_tutorial",
               SERIES_ID = "ABC_change_balance", # name of the series ID
               time_units = c("d", "d"), # in/out time units for pdf plots
               COMPO_MASTER = "0_CPS_MASTER_changing_balance.xlsx",
               plot_HIDE_BOXES_delta = c("SINK"), # hide in delta plots
               plot_HIDE_BOXES_size = c("SOURCE", "SINK"), # hide in size plots
               EACH_RUN_DIGEST = FALSE, # export the DIGEST for each run
               to_CPS_DIGEST_CSVs = TRUE) # export whole model to CSVs
```

`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, save_run_outputs = 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`	Edits csv outputs to the RUN DIGEST folder (logical, default is FALSE)
`save_run_outputs`	*OPTIONAL* Logical value. Allows saving all run outputs to directory containing INPUT file. By default, run outputs are stored in a temporary directory and are erased if not exported. 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.

By default (unless save_run_outputs = TRUE), run outputs are stored in the temporary directory and are not exported.

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_evS + 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***)

`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,
  plot_results = TRUE,
  save_run_outputs = FALSE
)
```

Arguments

workdir	Working directory of ***0_ISOBXR_MASTER.xlsx*** master file and where output files will be stored if exported by user. (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 among 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.

`plot_results` *OPTIONAL*
Logical value.
If TRUE, plots in R session the single model run evolution of delta values and box sizes for all boxes.
Default is TRUE.

`save_run_outputs`
OPTIONAL
Logical value.
Allows saving all run outputs to working directory (workdir).
By default, run outputs are stored in the temporary directory and are erased if not exported.
Default is FALSE.

Value

Calculates the time evolution of delta values and box sizes in all boxes.

run_isobxr returns by default a plot showing time evolution of delta values and box sizes for all boxes (set plot_results = FALSE to mute the plots).

run_isobxr creates a series of isotope data and metadata, all of which are stored in a temporary directory.
The user can save all outputs described below to their working directory by setting save_run_outputs = TRUE (default is FALSE).

If run_isobxr is run independently, it creates and stores all outputs in a *SERIES* folder, with the following name structure:
2_RUN + SERIES_ID

run_isobxr base workflow:

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 mass 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 for all balanced boxes, 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.
(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

1. 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***)

2. 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.

Examples

```
# Example 1. {ABC}, closed, balanced
# for more information see tutorial at
# https://ttacail.github.io/isobxr_web/vgn_04_Run_isobxr_tutorial.html#22_Run_the_model
```

```
# This is an example using the tutorial files embedded in package data
# It can be run as such.
run_isobxr(workdir = "/Users/username/Documents/1_ABC_tutorial",
           SERIES_ID = "ABC_closed_balanced", # series ID of the set of runs
           flux_list_name = "Fx1_ABC_closed_bal", # which flux list from FLUXES sheet
           coeff_list_name = "a1", # which coefficients list from COEFFS sheet
           t_lim = 2500, # how long do I want to run
           nb_steps = 250, # how many steps over this run duration
           time_units = c("d", "yr"), # run time units (days), plot time units (years)
           to_DIGEST_evD_PLOT = TRUE,
           to_DIGEST_CSV_XLS = TRUE,
           to_DIGEST_DIAGRAMS = TRUE) # export plot as pdf
```

`shinobxr_app` *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

```
shinobxr_app()
```

Value

No return value, called for launch of the html based shiny app.

`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,
  plot_results = TRUE,
  save_run_outputs = FALSE
)
```

Arguments

workdir	Working directory of ***0_ISOBXR_MASTER.xlsx*** master file, of the dynamic sweep master file (e.g., ***0_EXPLO_DYN_MASTER.xlsx***) and where output files will be stored if saved by user. (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 among 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.
plot_results	*OPTIONAL* Logical value. If TRUE, plots in R session the evolution of deltas as a function of time with respect to parameters 1 and 2, for all system finite boxes. Default is TRUE.
save_run_outputs	*OPTIONAL* Logical value.

Allows saving all run outputs to working directory (workdir).
By default, run outputs are stored in the temporary directory and are erased if not saved.
Default is FALSE.

Value

Calculates the delta values and box sizes at final state of the sweeping of 2D space of parameters in all boxes.

`sweep_dyn` returns by default a plot showing time evolution of delta values of the isotope composition of each finite box in the 2D space defined by the two swept parameters (set plot_results = FALSE to mute the plots).

The graphical results of the sweep can be also interactively explored using the `shinobxr_app` function in case user saves the outputs to the working directory (save_run_outputs = TRUE).

`sweep_steady` creates a series of isotope data and metadata, all of which are stored in a temporary directory.
The user can save all outputs described below to their working directory by setting save_run_outputs = TRUE (default is FALSE).

`sweep_dyn` creates and stores all outputs in a dedicated SERIES directory with the following name structure:
4_DYN + SERIES_ID + YYY, where YYY is a sweep dynamic run number automatically set between 001 and 999.
No overwriting of previous sweep dynamic run runs is possible.

`sweep_steady` base workflow:

1. Calculates the number of single runs the sweeping will require depending on the swept 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***

For examples, see https://ttacail.github.io/isobxr_web/vgn_08_sweep_dyn.html#4_Tutorial_example

---

`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.

Usage

```
sweep_steady(
  workdir,
  SERIES_ID,
  time_units,
  EXPLO_MASTER,
  EXPLO_AXIS_1,
  EXPLO_AXIS_2,
  to_STD_DIGEST_CSVs = FALSE,
  plot_results = TRUE,
  save_run_outputs = 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 if exported by user. (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 among 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.

`plot_results` *OPTIONAL*
Logical value.
If TRUE, plots in R session the heatmaps of delta values of all system finite boxes in the 2D space of swept parameters.
Default is TRUE.

`save_run_outputs`
OPTIONAL
Logical value.
Allows saving all run outputs to working directory (workdir).
By default, run outputs are stored in the temporary directory and are erased if not saved.
Default is FALSE.

Value

Calculates the delta values and box sizes at final state of the sweeping of 2D space of parameters in all boxes.

`sweep_steady` returns by default a heatmap plot of the isotope composition of each finite box in the 2D space defined by the two swept parameters (set plot_results = FALSE to mute the plots).

The graphical results of the sweep can be also interactively explored using the `shinobxr_app` function in case user saves the outputs to the working directory (save_run_outputs = TRUE).

`sweep_steady` creates a series of isotope data and metadata, all of which are stored in a temporary directory.
The user can save all outputs described below to their working directory by setting save_run_outputs = TRUE (default is FALSE).

`sweep_steady` creates and stores all outputs in a dedicated SERIES directory with the following name structure:
4_STD + SERIES_ID + YYY, where YYY is a sweep steady run number automatically set between 001 and 999.
No overwriting of previous sweep steady run runs is possible.

`sweep_steady` base workflow:

1. Calculates the number of single runs the sweeping will require depending on the swept parameters.
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 ***0_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***

For examples, see: https://ttacail.github.io/isobxr_web/vgn_07_sweep_steady.html#4_Tutorial_example

Index