Package 'isobxr'

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Type Package

Title Stable Isotope Box Modelling in R

Version 2.0.0

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. The mathematical models used in this package 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

Imports stringr, readxl, dplyr, data.table, deSolve, rlang (>= 0.4.11), grid, ggplot2, ggrepel, qgraph, writexl, R.utils, fs, magrittr, tidyr, gridExtra, purrr, reshape2, tictoc

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VignetteBuilder knitr

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Author Theo Tacail [aut, cre]

Maintainer Theo Tacail <theo.tacail@protonmail.com>

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Contents

`fit.final_space` *Fit n parameters to observations*

Description

A function to find the combinations of values of n parameters producing final state delta values fitting within confidence intervals of observations.

Usage

```
fit.final_space(
  workdir,
  obs_file_name,
  sweep_space_digest_folders,
  fit_name = NULL,
  output_dir = NULL,
  delta_reference_box = NaN,
  excluded_boxes = NULL,
  print_correlogram = FALSE,
  print_lda = FALSE,
  print_LS_surfaces = FALSE,
  parameter_subsets = NULL,
  custom_expressions = NULL,
  save_outputs = FALSE,
  export_fit_data = 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)

`obs_file_name` Name of csv file containing observations with csv extension. Stored in workdir. Example: "observations.csv" Should contain the following columns:

1. **BOX_ID**: BOX ID (e.g., A, OCEAN...) as defined in isobxr master file.
2. **delta.def** definition of delta value, e.g., d18O
3. **delta.ref** BOX_ID of reservoir used as a reference.
4. **obs.delta** average observed delta numerical value
5. **obs.CI** confidence interval of delta value
6. **obs.CI.def** definition of confidence interval, e.g., 95
7. **obs.file** name of data source file

`sweep_space_digest_folders` Name of sweep.final_nD digest directory. Should start with "4_FINnD" and end with "_digest"

`fit_name` Name given to specific fit. If NULL, output are named after date and time of fit.

`output_dir` Destination directory for fit outputs. If NULL, outputs are stored in sweep_space_digest_folders directory. Default is NULL.

`delta_reference_box` BOX ID of reference box, used to calculate difference between any box delta and reference box delta. Default is NaN. delta_reference_box should match at least one of the values declared in the delta.ref column of observation csv file.

`excluded_boxes` list of boxes to exclude from fit. Default is NULL.

`print_correlogram` If TRUE, includes correlograms to final report when applicable. Default is FALSE.

`print_lda` If TRUE, includes linear discriminant analysis to final report when applicable. Default is FALSE.

`print_LS_surfaces` If TRUE, includes surfaces of least squarred residuals to final report when applicable. Default is FALSE.

`parameter_subsets` List of limits vectors for parameters to subset before fit. For instance: list(swp.A.A_B = c(1, 1.00001)) to subset the swept fractionation factor from box A to B between 1 and 1.00001.

`custom_expressions` Vector of expressions to add to the list of fitted parameters. For instance: c("m0.A/f.A_B") to add the ratios of mass of A over A to B flux to the list of parameters.

`save_outputs` If TRUE, saves all run outputs to local working directory (workdir).
By default, run outputs are stored in a temporary directory and erased if not saved. Default is FALSE.

`export_fit_data`
If TRUE, exports fitted data as csv and rds files.

Value

A observation fit graphical report, in R session or exported as pdf, and a data report as R list or xlsx if required.

`merge_FINnD_chunks` *Merge results from all chunks of a given sweep.final_nD run*

Description

Merge results from all chunks of a given sweep.final_nD run

Usage

```
merge_FINnD_chunks(workdir, FINnD_digest_dir.to_merge, save_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)

`FINnD_digest_dir.to_merge`
Name of sweep.final_nD digest directory to which current chunks should be merged.
For instance: "4_FINnD_0_SWEEP_FINnD_demo_001_000_digest"

`save_outputs` If TRUE, saves merged chunks outputs to sweep.final_nD digest directory.

Value

Merged chunks sweep.final_nD outputs, including results, chunk logs, chunked parameter spaces.

plot_dyn_2D *plot sweep.dyn_2D outputs*

Description

A function to plot delta vs time from the sweep.dyn_2D runs

Usage

```
plot_dyn_2D(
  workdir,
  sweep_dir_name,
  time_unit = NULL,
  time_range = NULL,
  hidden_boxes = NULL,
  return_as_print = TRUE,
  free_y_scale = TRUE,
  swap_sweep_params = FALSE,
  show.delta_drift = FALSE,
  time_as_log10 = TRUE
)
```

Arguments

workdir	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
sweep_dir_name	Full name of sweep.dyn_2D SERIES directory (character string)
time_unit	Time unit to use on plot if different from native time unit. Character string, to be selected among the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* Default is NULL.
time_range	Time range to zoom on as vector of two values, such as: c(0,100) Values in displayed time units. Default is NULL.
hidden_boxes	List of boxes to hide from plots, as a vector of character strings. For instance c("SOURCE", "SINK"). Default is NULL.
return_as_print	If TRUE, prints delta and size vs. time plots in a single page figure on R. If FALSE, returns separately delta and size vs. time plots as list of editable R objects. Default is TRUE.
free_y_scale	If TRUE, frees Y axis scale. Default is TRUE.

swap_sweep_params
: If TRUE, swaps the sweep parameter 1 and 2 representations from color to facet scales.
Default is FALSE.

show.delta_drift
: If TRUE, displays drift of delta values from t0.

time_as_log10
: If TRUE, uses logarithmic time scale in plot.
Default is TRUE.

Value

A set of plots showing the evolution of delta and sizes with time.

`plot_relaxation` *plot relaxation*

Description

A function to plot the relaxation of isotope ratios in a system, including characteristic times

Usage

```
plot_relaxation(
  workdir,
  flux_list,
  coeff_list,
  spiked_boxes,
  spike.max_delta = 100,
  n_steps = 10000,
  hidden_boxes = NULL,
  show.residence_time = TRUE,
  show.facets = FALSE,
  time_landmarks = NULL,
  time_as_log10 = TRUE,
  isobxr_master_file = "0_ISOBXR_MASTER",
  time.resolution_cut = NULL
)
```

Arguments

workdir
: Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)

flux_list
: 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 ***isobxr excel master file***.
(character string)

`coeff_list` 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 ***isobxr excel master file***.
(character string)

`spiked_boxes` Vector of box names ("BOX_ID") to be spiked.
If several boxes are listed, initial spike will be evenly distributed from 0 to spike.max_delta value.

`spike.max_delta`
Value of the maximum spike isotope composition
(in permil on the delta scale).
Default is 100 permil.

`n_steps` Number of calculation steps. Determines the resolution of the run.
Default is 10000.

`hidden_boxes` Vector of boxes to hide from plots.
For instance c("SOURCE", "SINK").
Default is NULL.

`show.residence_time`
If TRUE, displays box-specific residence times on plot.
Default is FALSE.

`show.facets` If TRUE, displays results in box-specific facets.
Default is FALSE.

`time_landmarks` Vector of time landmarks to display on x-axis (numerical values).

`time_as_log10` If TRUE, uses logarithmic time scale in plot.
Default is TRUE.

`isobxr_master_file`
Name of ***isobxr excel master file***.
Default is "0_ISOBXR_MASTER".

`time.resolution_cut`
Time below which resolution is increased. Default is NULL.

Value

A plots showing the evolution of the isotopic ratios in the system until full relaxation, defined as the maximum relaxation time multiplied by 10.

Examples

```
## Not run:
plot_relaxation(workdir = "/Users/username/Documents/1_ABC_tutorial",
                flux_list = "Fx6_ABC_open_bal",
                coeff_list = "a0",
                n_steps = 1000,
                spiked_boxes = c("SOURCE"))

## End(Not run)
```

plot_scenario *plot sim.scenario outputs*

Description

A function to plot delta and size vs time from the sim.scenario runs and to include observations along simulations.

Usage

```
plot_scenario(
  workdir,
  scenario_dir_name,
  shown_runs = NULL,
  time_unit = NULL,
  hidden_boxes = NULL,
  return_as_print = TRUE,
  show.facets = FALSE,
  show.run_separations = TRUE,
  observations_file = NULL,
  observations_groups = NULL
)
```

Arguments

workdir	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
scenario_dir_name	name of sim.scenario SERIES directory (starts with 3_SCEN)
shown_runs	Vector of successive run numbers (RUN_n) to be displayed (e.g., 1:5). Default is run 2 to last run (hides initial relaxation run)
time_unit	Time unit to use on plot if different from native time unit. Character string, to be selected among the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* Default is NULL.
hidden_boxes	List of boxes to hide from plots, as a vector of character strings. For instance c("SOURCE", "SINK").
return_as_print	If TRUE, prints delta and size vs. time plots in a single page figure on R. If FALSE, returns separately delta and size vs. time plots as list of two editable R objects.
show.facets	If TRUE, shows delta vs. time as faceted by BOX. Default is FALSE.
show.run_separations	If TRUE, shows limits between subruns. Default is TRUE.

`observations_file`
: Name of the csv file containing observations (without csv extension).
Observation csv file should contain the following columns:

1. **GROUP**: observation subset group label if relevant
2. **BOX_ID**: BOX ID (e.g., A, OCEAN...) as defined in isobxr master file.
3. **delta.def** definition of delta value, e.g., d18O
4. **obs.delta** average observed delta numerical value
5. **obs.CI** confidence interval of delta value
6. **obs.CI.def** definition of confidence interval, e.g., 95
7. **obs.counts** number of observations corresponding to average delta
8. **Time** time of observation in scenario timeline, in display time units

Default is NULL.

`observations_groups`
: vector of observations groups to include in plot,
from GROUP column in observation csv file.
Default is NULL.

Value

A set of plots showing the evolution of delta and sizes with time.

`plot_single_run` *plot sim.single_run outputs*

Description

A function to plot delta and size vs time from the sim.single_run outputs

Usage

```
plot_single_run(
  workdir,
  RUN_ID,
  time_as_log10 = TRUE,
  time_unit = NULL,
  hidden_boxes = NULL,
  return_as_print = TRUE
)
```

Arguments

`workdir`	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
`RUN_ID`	ID of the run (formerly SERIES_RUN_ID). Corresponds to the name of the .rds file storing the results of the run.

`time_as_log10` If TRUE, uses logarithmic time scale in plot.
Default is TRUE.

`time_unit` Time unit to use on plot if different from native time unit.
Character string, to be selected among the following:
micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr
Default is NULL.

`hidden_boxes` List of boxes to hide from plots, as a vector of character strings.
For instance c("SOURCE", "SINK").

`return_as_print`
If TRUE, prints delta and size vs. time plots in a single page figure on R.
If FALSE, returns separately delta and size vs. time plots as list of editable R objects.
Default is TRUE.

Value

A set of plots showing the evolution of delta and sizes with time.

`read.dyn_2D_master` *Read and inspect sweep.dyn_2D master files*

Description

A function to read and inspect the sweep.dyn_2D master files and obtain a master formatted list.

Usage

```
read.dyn_2D_master(workdir, dyn_2D_master_file, isobxr_master_file)
```

Arguments

`workdir` Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)

`dyn_2D_master_file`
Name of ***sweep.dyn_2D excel master file***. (without file "xlsx" extension).

`isobxr_master_file`
Name of ***isobxr excel master file***. (without file "xlsx" extension). Default is "0_ISOBXR_MASTER".

Value

List of formatted dyn_2D_master_file master inputs.

Examples

```
read.dyn_2D_master(workdir = "/Users/username/Documents/1_ABC_tutorial",
                   dyn_2D_master_file = "0_SWEEP_DYN_demo",
                   isobxr_master_file = "0_ISOBXR_MASTER")
```

`read.final_nD_master` *Read and inspect sweep.final_nD master files*

Description

A function to read and inspect the sweep.final_nD master files and obtain a master formatted list.

Usage

```
read.final_nD_master(workdir, final_nD_master_file, isobxr_master_file)
```

Arguments

`workdir`	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
`final_nD_master_file`	Name of ***sweep.final_nD excel master file***. (without file "xlsx" extension).
`isobxr_master_file`	Name of ***isobxr excel master file***. (without file "xlsx" extension). Default is "0_ISOBXR_MASTER".

Details

List contains:

1. **param_space** data frame of shuffled all combinations of all parameters values.
2. **sweep.DEFAULT** data frame of default run conditions
   (flux and coeff lists, t_max, chunk size)
3. **sweep_lists_ids** list of names of swept parameters

Value

List of formatted sweep.final_nD master inputs

Examples

```
read.final_nD_master(workdir = "/Users/username/Documents/1_ABC_tutorial",
                     final_nD_master_file = "0_SWEEP_FINnD_demo",
                     isobxr_master_file = "0_ISOBXR_MASTER")
```

`read.isobxr_master` *Read and inspect isobxr master files*

Description

A function to read and inspect the isobxr master files and obtain a master formatted list.

Usage

```
read.isobxr_master(
  workdir,
  isobxr_master_file = "0_ISOBXR_MASTER",
  inspect = TRUE,
  export_rds = FALSE
)
```

Arguments

`workdir`	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
`isobxr_master_file`	Name of ***isobxr excel master file***. (without file "xlsx" extension). Default is "0_ISOBXR_MASTER".
`inspect`	If TRUE, checks all inputs from isobxr master file for format and structure errors. Default is TRUE.
`export_rds`	If TRUE, exports rds version of isobxr master file to working directory. Default is FALSE.

Value

A formatted list of data frames containing constants, box, fluxes and fractionation coefficients descriptions.

Examples

```
read.isobxr_master(workdir = "/Users/username/Documents/1_ABC_tutorial",
                   isobxr_master_file = "0_ISOBXR_MASTER",
                   export_rds = FALSE,
                   inspect = TRUE)
```

read.scenario_master *Read and inspect scenario master files*

Description

A function to read and inspect the scenario master files and obtain a master formatted list.

Usage

```
read.scenario_master(
  workdir,
  scenario_master_file,
  isobxr_master_file = "0_ISOBXR_MASTER"
)
```

Arguments

workdir	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)
scenario_master_file	Name of ***scenario excel master file***. (without file "xlsx" extension).
isobxr_master_file	Name of ***isobxr excel master file***. (without file "xlsx" extension). Default is "0_ISOBXR_MASTER".

Value

List of formatted scenario master inputs.

Examples

```
read.scenario_master(workdir = "/Users/username/Documents/1_ABC_tutorial",
                     scenario_master_file = "0_SCENARIO_source_change",
                     isobxr_master_file = "0_ISOBXR_MASTER")
```

sim.scenario *Simulate a scenario*

Description

A function to compose an isotope box model scenario, defined by a series of 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

```
sim.scenario(
  workdir,
  SERIES_ID,
  scenario_master_file,
  isobxr_master_file = "0_ISOBXR_MASTER",
  plot.hidden_boxes = NULL,
  plot.time_unit = NULL,
  export.single_run_digests = FALSE,
  export.data_as_csv_xlsx = FALSE,
  show.delta_plot = TRUE,
  save_outputs = FALSE,
  inspect_inputs = TRUE
)
```

Arguments

`workdir`	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user.
`SERIES_ID`	Name of the series the scenario run belongs to. It determines the folder in which the output files will be stored inside workdir.
`scenario_master_file`	Name of ***scenario excel master file***.
`isobxr_master_file`	Name of ***isobxr excel master file***. Default is "0_ISOBXR_MASTER".
`plot.hidden_boxes`	list of box names (BOX_ID) to hide in scenario plot.
`plot.time_unit`	Time unit to use on plot if different from native time unit. Character string, to be selected among the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* Default is NULL.

`export.single_run_digests`
: If TRUE, exports full digest of each single run of the scenario. Default is FALSE.

`export.data_as_csv_xlsx`
: If TRUE, exports full scenario result data as csv and xlsx fo full to scenario digest directory.
Default is FALSE.

`show.delta_plot`
: If TRUE, prints delta and size time evolution plots in R.
Default is TRUE.

`save_outputs`
: If TRUE, saves all run outputs to local working directory (workdir).
By default, run outputs are stored in a temporary directory and erased if not saved.
Default is FALSE.

`inspect_inputs`
: If TRUE, inspects and proof checks format of input taken from ***isobxr excel master file***.
(Inspection run by `read.isobxr_master` function.)
Default is TRUE.

Value

Delta values and box sizes as a function of time.
sim.scenario outputs are saved to workdir if save_outputs = TRUE.

sim.scenario outputs consist of

1. **single run results** in SERIES directory: all single runs results as rds files
2. **scenario digest** in scenario DIGEST directory (SERIES/DIGEST):
   (a) **isobxr master file archive** as xlsx
   (b) **scenario master file archive** as xlsx
   (c) **plot of delta and size vs. time** as pdf
   (d) **scenario results data set** as rds, containing:
      i. **delta_vs_t** data frame of delta as a function of time
      ii. **size_vs_t** data frame of box sizes as a function of time
      iii. **scenario_master** list containing all inputs from scenario master file
      iv. **scenario_log** data frame of scenario specific LOG excerpt
      v. **isobxr_master** list containing all inputs from isobxr master file
      vi. **paths** list of scenario specific paths

Examples

```
## Not run:
sim.scenario(workdir = "/Users/username/Documents/1_ABC_tutorial",
             SERIES_ID =  "1_source_change",
             scenario_master_file = "0_SCENARIO_source_change",
             isobxr_master_file = "0_ISOBXR_MASTER")

## End(Not run)
```

`sim.single_run` *Run a single isotope box-model simulation*

Description

A function to run the isobxr stable isotope box model, assessing the design of the model and automatically running `solve_numerically` or `solve_analytically` depending on system design.

Usage

```
sim.single_run(
  workdir,
  SERIES_ID,
  flux_list,
  coeff_list,
  t_max,
  n_steps,
  isobxr_master_file = "0_ISOBXR_MASTER",
  suppress_messages = FALSE,
  export.diagrams = FALSE,
  export.delta_plot = FALSE,
  export.data_as_csv_xlsx = FALSE,
  plot.time_as_log10 = TRUE,
  plot.time_unit = NULL,
  show.delta_plot = TRUE,
  inspect_inputs = TRUE,
  save_outputs = FALSE,
  return_data = FALSE,
  solver = "auto",
  n_zeros_RUN_IDs = 4,
  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,
  isobxr_master = NULL,
  diagram_pdf.widh_height = NULL
)
```

Arguments

`workdir`	Working directory of ***isobxr excel master file*** and where output files will be stored if exported by user. (character string)

`SERIES_ID` Name of the series the run belongs to.
It determines the folder in which the output files will be stored inside workdir.
(character string)

`flux_list` 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 ***isobxr excel master file***.
(character string)

`coeff_list` 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 ***isobxr excel master file***.
(character string)

`t_max` Run duration, given in the same time units as unit declared in **CONSTANTS** spreadsheet of ***isobxr excel master file*** in the **TIME_UNIT** column. (integer)

`n_steps` Number of calculation steps.
It determines the resolution of the run.
(integer)

`isobxr_master_file`
Name of ***isobxr excel master file***.
Default is "0_ISOBXR_MASTER".

`suppress_messages`
If TRUE, hides all information and warning messages regarding run.
Default is FALSE.

`export.diagrams`
If TRUE, exports box-model flux and fractionation diagrams as pdf.
Default is FALSE.

`export.delta_plot`
If TRUE, exports delta and size time evolution plots of the evolution of the system, as pdf.
Default is FALSE.

`export.data_as_csv_xlsx`
If TRUE, exports all results and run conditions as csv and xlsx files,
to DIGEST directory.
Default is FALSE.

`plot.time_as_log10`
If TRUE, uses logarithmic time scale in plot.
Default is FALSE.

`plot.time_unit` Time unit to use on plot if different from native time unit.
Character string, to be selected among the following:
micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr
Default is NULL.

`show.delta_plot`
If TRUE, prints delta and size time evolution plots in R. Default is TRUE.

`inspect_inputs` If TRUE, inspects and proof checks format of input taken from ***isobxr excel master file***.
(Inspection run by `read.isobxr_master` function.)
Default is TRUE.

`save_outputs` If TRUE, saves all run outputs to local working directory (workdir).
By default, run outputs are stored in a temporary directory and erased if not saved.
Default is FALSE.

`return_data` If TRUE, returns all data (inputs and outputs) as a list.
Default is FALSE.

`solver` Determines what solver to used: "analytical" or "numerical".
Default is "auto" for automatic selection of adapted solver. Note that this option returns warnings or prevents user to run when solver wished is not adapted to system solution.

`n_zeros_RUN_IDs`
Number of figures used in iteration of RUNs of a given series (SERIES_ID).
Default is 4: the run IDs of a given series range between 0001 and 9999.

`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 ***isobxr excel master 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 ***isobxr excel master 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 ***isobxr excel master file***.
Dataframe formatting details are in isobxr vignette.
Default is NULL.

`COMPOSITE` *NOT TO BE USED IN SINGLE RUN*
Logical value automatically defined in `sim.scenario`.
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 sim.scenario.
Default is NaN.

COMPO_SERIES_FAMILY
NOT TO BE USED IN SINGLE RUN
Composite run series family, automatically defined in sim.scenario.
Default is NaN.

EXPLORER *NOT TO BE USED IN SINGLE RUN*
Logical value automatically defined in sweep.final_nD or sweep.dyn_2D.
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.final_nD or sweep.dyn_2D.
Default is NaN.

EXPLO_SERIES_FAMILY
NOT TO BE USED IN SINGLE RUN
Sweep run series family, automatically defined in sweep.final_nD or sweep.dyn_2D.
Default is NaN.

isobxr_master isobxr_master list of input dataframes formatted by read.isobxr_master
Overwrites isobxr_master_file. Default is NULL.

diagram_pdf.widh_height
Vector of width and height in inches of the pdf diagrams.

Value

A results data set as a list containing the following components:

1. **inputs** input data:
   (a) **CONSTS** data frame of all run specific constants.
   (b) **INITIAL** data frame of delta and sizes at t = 0 in all boxes.
   (c) **FLUXES** data frame of all fluxes intensities (row ID: FROM / col ID: TO)
   (d) **COEFFS** data frame of all fractionation coefficient values (row ID: FROM / col ID: TO)
   (e) **BOX_META** data frame of box specific metadata (e.g., flux balance, residence times, layout position)
   (f) **bx.groups** list of box names grouped by relevant categories (e.g., disconnected boxes, infinite boxes)
   (g) **LOG** data frame of run specific LOG excerpt.
2. **outputs** output data:
   (a) **solver**
   (b) **final_state**
   (c) **delta_vs_t**
   (d) **size_vs_t**
   (e) **for analytical solutions**
      i. **diffeq_solutions** solutions of differential equations, including relaxation times, eigenvalues, constants, eigenvectors
3. **paths** list of run specific paths

Examples

```
## Not run:
sim.single_run(workdir = "/Users/username/Documents/1_ABC_tutorial",
               SERIES_ID = "1_ABC_balanced_closed",
               flux_list = "Fx1_ABC_bal",
               coeff_list = "a1",
               t_max = 2500,
               n_steps = 2500)

## End(Not run)
```

`solve_analytically` *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 manual use.
The analytical solver finds the eigenvalues and eigenvectors of the ODES.
It determines the set of analytical solutions that describes the evolution of isotope ratios in each box over time.

Usage

```
solve_analytically(IN, paths, to_DIGEST_csv = FALSE, return_results = FALSE)
```

Arguments

`IN`	input data, edited by `sim.single_run` (list of dataframes)
`paths`	paths object edited by `sim.single_run` (list of characters)
`to_DIGEST_csv`	if TRUE, edits csv outputs to DIGEST directory Default is FALSE.
`return_results`	if TRUE, results returned as a list of R objects. Default is FALSE.

Value

Analytically determined evolution of stable isotope compositions in all boxes over the run duration as specified in INPUT file.

Run outputs are stored in a temporary directory and not exported by `solve_numerically`.

The outputs of the run are stored in the rds output file in the SERIES directory with the following file name structure:
SERIES_ID + RUN_n.rds

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 + SERIES_ID + RUN_n + .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 + SERIES_ID + RUN_n + .csv***)
3. evD data file of the evolution with time of the delta values in all boxes.
   (file name structure: ***out_3_A_evD + SERIES_ID + RUN_n + .csv***)

`solve_numerically` *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 manual use.
The numerical solver uses the ***deSolve::ode*** function to integrate the stable isotopes ratios over time in each box. It allows the calculation of the evolution of stable isotope ratio 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

```
solve_numerically(IN, paths, to_DIGEST_csv = FALSE, return_results = FALSE)
```

Arguments

`IN`	input data, edited by `sim.single_run` (list of dataframes)
`paths`	paths object edited by `sim.single_run` (list of characters)
`to_DIGEST_csv`	if TRUE, edits csv outputs to DIGEST directory Default is FALSE.
`return_results`	if TRUE, results returned as a list of R objects. Default is FALSE.

Value

Numerically determined evolution of stable isotope compositions
and masses of element X in all boxes over the run duration as specified in INPUT file.

Run outputs are stored in a temporary directory and not exported by `solve_numerically`.

The outputs of the run are stored in the rds output file in the SERIES directory with the following file name structure:
SERIES_ID + RUN_n.rds

Optional csv outputs to DIGEST directory 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***)

`sweep.dyn_2D` *Sweep the space of two parameters during the response to a perturbation*

Description

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

Usage

```
sweep.dyn_2D(
  workdir,
  SERIES_ID,
  plot.time_unit = NULL,
  isobxr_master_file = "0_ISOBXR_MASTER",
  sweep_master_file,
  swept_param_1,
  swept_param_2,
  export.data_as_csv_xlsx = TRUE,
  show.delta_plot = TRUE,
  save_outputs = FALSE,
  ask_confirmation = TRUE,
  keep_single_run_rds = 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 belongs to. It determines the folder in which the output files will be stored inside workdir. (character string)
`plot.time_unit`	Time unit to use on plot if different from native time unit. Character string, to be selected among the following: *micros, ms, s, min, h, d, wk, mo, yr, kyr, Myr, Gyr* Default is NULL.

`isobxr_master_file`
: Name of ***isobxr excel master file***.
Default is "0_ISOBXR_MASTER".

`sweep_master_file`
: Name of ***sweep.dyn_2D excel master file***. (without file "xlsx" extension).

`swept_param_1`
: Set of values of sweeping parameter 1.
Formatted data frame, see vignette for further details.

`swept_param_2`
: Set of values of sweeping parameter 2.
Formatted data frame, see vignette for further details.

`export.data_as_csv_xlsx`
: If TRUE, exports full sweep result data as csv and xlsx fo full to sweep digest directory.
Default is TRUE.

`show.delta_plot`
: If TRUE, prints delta and size time evolution plots in R.
Default is TRUE.

`save_outputs`
: If TRUE, saves all run outputs to local working directory (workdir).
By default, run outputs are stored in a temporary directory and erased if not saved.
Default is FALSE.

`ask_confirmation`
: If TRUE, asks confirmation to run in interactive sessions.
Default is TRUE.

`keep_single_run_rds`
: If TRUE, keeps single runs outputs (rds files in SERIES directory).
Default is FALSE.

Value

Delta values and box sizes as a function of time in response to a perturbation, in a 2D space of parameters sweep.dyn_2D outputs are saved to workdir if save_outputs = TRUE.

sweep.dyn_2D outputs consist of

1. **single run results** in SERIES directory: all single runs results as rds files (keep_single_run_rds = TRUE)
2. **sweep digest** in sweep DIGEST directory (SERIES/DIGEST):
   (a) **isobxr master file archive** as xlsx (export.data_as_csv_xlsx = TRUE)
   (b) **sweep.dyn_2D master file archive** as xlsx (export.data_as_csv_xlsx = TRUE)
   (c) **sweep.dyn_2D LOG excerpt** as csv (export.data_as_csv_xlsx = TRUE)
   (d) **delta_size_vs_t** csv of delta and size vs time in 2D space (export.data_as_csv_xlsx = TRUE)
   (e) **plot of delta and size vs. time in 2D space** as pdf
   (f) **sweep.dyn_2D results data set** as rds, containing:
      i. **delta_size_vs_t** data frame of delta and size as a function of time
      ii. **sweeep_master** list containing all inputs from sweep master file

iii. **sweep_log** data frame of sweep specific LOG excerpt
iv. **isobxr_master** list containing all inputs from isobxr master file
v. **paths** list of sweep specific paths

Examples

```
## Not run:
sweep.dyn_2D(workdir = "/Users/username/Documents/1_ABC_tutorial",
             SERIES_ID = "sweep_dyn_test",
             isobxr_master_file = "0_ISOBXR_MASTER",
             sweep_master_file = "0_SWEEP_DYN_demo",
             swept_param_1 = data.frame(FROM = c("A"),
                                        TO = c("C"),
                                        ALPHA_MIN = 0.999,
                                        ALPHA_MAX = 1,
                                        ALPHA_STEPS = 0.0005,
                                        EXPLO_TYPES = "EXPLO_1_ALPHA"),
             swept_param_2 = data.frame(BOX_ID = c("B"),
                                        SIZE_MIN = 2100,
                                        SIZE_MAX = 3000,
                                        SIZE_STEPS = 300,
                                        EXPLO_TYPES = "EXPLO_1_SIZE"),
             ask_confirmation = FALSE)

## End(Not run)
```

`sweep.final_nD` *Sweep the space of n parameters at the final state of a system*

Description

A function to assess the influence of n parameters (varying over a range of values) on the final state of a system.

Usage

```
sweep.final_nD(
  workdir,
  sweep_master_file,
  sweep_dir_to_complete = NULL,
  export.data_as_csv_xlsx = FALSE,
  isobxr_master_file = "0_ISOBXR_MASTER",
  save_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)
`sweep_master_file`	Name of ***sweep.final_nD excel master file***. (without file "xlsx" extension).
`sweep_dir_to_complete`	Name of directory of previously halted sweep.final_nD run that the user wishes to continue. Starts with "4_FINnD". Default is NULL.
`export.data_as_csv_xlsx`	If TRUE, exports chunk sweep result data as csv and xlsx fo full to chunk digest directory. Default is FALSE.
`isobxr_master_file`	Name of ***isobxr excel master file***. Default is "0_ISOBXR_MASTER".
`save_outputs`	If TRUE, saves all run outputs to local working directory (workdir). By default, run outputs are stored in a temporary directory and erased if not saved. Default is FALSE.

Value

Delta values and box sizes at final state of the system, in the n-dimensions space of parameters. sweep.final_nD outputs are saved to workdir if save_outputs = TRUE.

sweep.final_nD outputs

1. **digest sweep.final_nD outputs** full sweep.final_nD outputs are stored in a digest directory directly in workdir:
   (a) **isobxr master file archive** as xlsx
   (b) **global chunk_log** as csv
   (c) **global chunk_log** as rds
   (d) **sweep.final_nD master file archive** as xlsx
   (e) **sweep.final_nD merged chunks LOG excerpt** as csv
   (f) **sweep.final_nD merged param_space**, current progress, as rds (space of swept parameters)
   (g) **sweep.final_nD merged results**, current progress, as rds
      i. data frame containing delta and size at final state across whole n-dimensions space of parameters
      ii. **sweep.final_nD param_space** as planned, as rds
      iii. **sweep.final_nD sweep_default** data frame of default run conditions, as rds
      iv. **sweep.final_nD sweep progress plot** as pdf, follows merging of chunks
2. **chunks sweep.final_nD outputs** chunk directories are edited in case total number. of runs exceeds chunk size defined in sweep.final_nD master file. They are removed after full sweep.

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