# Package 'shelltrace'

October 14, 2022

Type Package Title Bivalve Growth and Trace Element Accumulation Model Version 3.5.1 Date 2017-09-27 Author Niels J. de Winter Maintainer Niels J. de Winter <niels.de.winter@vub.be> **Depends** R (>= 3.1.0) Imports xlsx, bmp, tiff, grDevices, stats Description Contains all the formulae of the growth and trace element uptake model described in the equallynamed Geoscientific Model Development paper (de Winter, 2017, <doi:10.5194/gmd-2017-137>). The model takes as input a file with X- and Y-coordinates of digitized growth increments recognized on a longitudinal cross section through the bivalve shell, as well as a BMP file of an elemental map of the cross section surface with chemically distinct phases separated by phase analysis. It proceeds by a step-by-step process described in the paper, by which digitized growth increments are used to calculate changes in shell height, shell thickness, shell volume, shell mass and shell growth rate through the bivalve's life time. Then, results of this growth modelling are combined with the trace element mapping results to trace the incorporation of trace elements into the bivalve shell. Results of various modelling parameters can be exported in the form of XLSX files. License GPL-3

## LazyData true

URL https://github.com/nielsjdewinter/ShellTrace,

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http://nidewint.wixsite.com/nielsdewinter

BugReports https://github.com/nielsjdewinter/ShellTrace/issues RoxygenNote 6.0.1

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# Index

BMP

BMP image of phase map of cross section of modern oyster.

## Description

An image of the microXRF phase map of the cross section used for this model from the Crassostre gigas #1 oyster used as an example in de Winter (2017)

# Usage

data(BMP)

# Format

A BMP image imported into R as a large data array

# Source

https://doi.org/10.5194/gmd-2017-137-supplement

cross\_section

#### Description

A dataset containing X- and Y-coordinates of digitized growth increments from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) resampled to fit the same X-axis.

#### Usage

data(cross\_section)

## Format

A data frame with 101 rows and 10 variables:

- 0 X-coordinates in mm
- 44 Empty column, title contains day of the year the shell started growing (estimated)
- **0** Y-coordinates of digitized increment 0 (top of shell), title contains age in days
- 30 Y-coordinates of digitized increment 1, title contains age in days
- 90 Y-coordinates of digitized increment 2, title contains age in days
- 270 Y-coordinates of digitized increment 3, title contains age in days
- 420 Y-coordinates of digitized increment 4, title contains age in days
- 780 Y-coordinates of digitized increment 5, title contains age in days
- 1050 Y-coordinates of digitized increment 6, title contains age in days
- 1290 Y-coordinates of digitized increment 7 (bottom of shell), title contains age in days

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

el\_time

Matrix listing the concentrations of elements in every subincrement

#### Description

A dataset containing the concentrations of every element measured in the phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017) reconstructed in every subincrement.

#### Usage

data(el\_time)

## image\_length

# Format

A data frame with 24 rows and 1291 variables:

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

image\_length Length (in mm) of the digitized phase map image.

# Description

A single value of the image length in mm

## Usage

data(image\_length)

#### Format

A single value: Length in mm of digitized shell cross section

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

IncG	Interpolated subincrements in cross section of modern oyster rescaled
	to the same X-axis.

## Description

A dataset containing X- and Y-coordinates of subincrements interpolated between digitized growth increments from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sampled to fit a common X-axis. A Xstep of 0.1, a Tstep of 1 and a growth season of 250 days are used.

#### Usage

data(IncG)

## Format

A large data frame with 101 rows and 1291 variables:

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

incr\_matrix0

#### Description

A dataset containing specific parameters calculated for all digitized growth increments from the Crassostre gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

data(incr\_matrix0)

#### Format

A data frame with 8 rows and 3 variables:

growth band name of the growth increment

age (days) Age associated with the deposition of the growth increment

**age\_cal (days)** Age associated with the deposition of the growth increment, calibrated to the seasonal cycle

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

incr_matrix1	Matrix containing data calculated	for each growth band.

# Description

A dataset containing specific parameters calculated for all digitized growth increments from the Crassostre gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

data(incr\_matrix1)

#### Format

A data frame with 8 rows and 5 variables:

growth band name of the growth increment

age (days) Age associated with the deposition of the growth increment

**age\_cal (days)** Age associated with the deposition of the growth increment, calibrated to the seasonal cycle

incr\_area area between subsequent increments

incr\_cumarea area between increment and the top of the shell

#### incr\_matrix2

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

incr\_matrix2 Matrix containing data calculated for each growth band.

#### Description

A dataset containing specific parameters calculated for all digitized growth increments from the Crassostre gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

```
data(incr_matrix2)
```

#### Format

A data frame with 8 rows and 6 variables:

growth band name of the growth increment

age (days) Age associated with the deposition of the growth increment

**age\_cal (days)** Age associated with the deposition of the growth increment, calibrated to the seasonal cycle

incr\_area area between subsequent increments

incr\_cumarea area between increment and the top of the shell

av\_thickness average thickness of area between increment and the top of the shell

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

incr\_matrix3 Matrix containing data calculated for each growth band.

## Description

A dataset containing specific parameters calculated for all digitized growth increments from the Crassostre gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

data(incr\_matrix3)

## lengthfactor

#### Format

A data frame with 8 rows and 11 variables:

growth band name of the growth increment

age (days) Age associated with the deposition of the growth increment

- **age\_cal (days)** Age associated with the deposition of the growth increment, calibrated to the seasonal cycle
- incr\_area area between subsequent increments
- incr\_cumarea area between increment and the top of the shell
- av\_thickness average thickness of area between increment and the top of the shell
- p1x X-value of first (leftmost) point in growth increment
- ply Y-value of first (leftmost) point in growth increment
- **p2x** X-value of last (rightmost) point in growth increment
- p2y Y-value of last (rightmost) point in growth increment
- shell\_height Height of shell during deposition of shell increment

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

lengthfactor	Multiplier used to convert shell cross section from pixels to mm
--------------	--

## Description

A single value of the amount of mm contained in one pixel

#### Usage

```
data(lengthfactor)
```

#### Format

A single value:

Length in mm of one pixel in the digitized shell cross section

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

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M\_el\_mat

#### Description

A dataset containing trace element accumulation modelled for every based on the a phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

# Usage

data(M\_el\_mat)

## Format

A data frame with 5 rows and 24 variables: C Mass accumulation of C in subincrement

O Mass accumulation of O in subincrement Na Mass accumulation of Na in subincrement Mg Mass accumulation of Mg in subincrement Al Mass accumulation of Al in subincrement Si Mass accumulation of Si in subincrement **P** Mass accumulation of P in subincrement S Mass accumulation of S in subincrement Cl Mass accumulation of Cl in subincrement K Mass accumulation of K in subincrement Ca Mass accumulation of Ca in subincrement Ti Mass accumulation of Ti in subincrement Cr Mass accumulation of Cr in subincrement Mn Mass accumulation of Mn in subincrement Fe Mass accumulation of Fe in subincrement Ni Mass accumulation of Ni in subincrement Cu Mass accumulation of Cu in subincrement **Zn** Mass accumulation of Zn in subincrement Br Mass accumulation of Br in subincrement **Rb** Mass accumulation of Rb in subincrement Sr Mass accumulation of Sr in subincrement **Rh** Mass accumulation of Rh in subincrement Ba Mass accumulation of Ba in subincrement Pb Mass accumulation of Pb in subincrement

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

M\_el\_mat\_c

## Description

A dataset containing mass accumulation of trace elements modelled for every based on the a phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

#### Usage

data(M\_el\_mat\_c)

## Format

A data frame with 5 rows and 24 variables:

C Cumulative mass accumulation of C in subincrement O Cumulative mass accumulation of O in subincrement Na Cumulative mass accumulation of Na in subincrement Mg Cumulative mass accumulation of Mg in subincrement Al Cumulative mass accumulation of Al in subincrement Si Cumulative mass accumulation of Si in subincrement **P** Cumulative mass accumulation of P in subincrement S Cumulative mass accumulation of S in subincrement Cl Cumulative mass accumulation of Cl in subincrement K Cumulative mass accumulation of K in subincrement **Ca** Cumulative mass accumulation of Ca in subincrement Ti Cumulative mass accumulation of Ti in subincrement Cr Cumulative mass accumulation of Cr in subincrement Mn Cumulative mass accumulation of Mn in subincrement Fe Cumulative mass accumulation of Fe in subincrement Ni Cumulative mass accumulation of Ni in subincrement Cu Cumulative mass accumulation of Cu in subincrement Zn Cumulative mass accumulation of Zn in subincrement Br Cumulative mass accumulation of Br in subincrement **Rb** Cumulative mass accumulation of Rb in subincrement Sr Cumulative mass accumulation of Sr in subincrement **Rh** Cumulative mass accumulation of Rh in subincrement **Ba** Cumulative mass accumulation of Ba in subincrement **Pb** Cumulative mass accumulation of Pb in subincrement

## O1\_input

# Source

https://doi.org/10.5194/gmd-2017-137-supplement

01\_input

Digitized growth increments in cross section of modern oyster.

#### Description

A dataset containing X- and Y-coordinates of digitized growth increments from the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

#### Usage

data(01\_input)

#### Format

A data frame with 181 rows and 26 variables:

x\_base X-coordinate in pixels of bottom line on image

**y\_base** Y-coordinate in pixels of bottom line on image, second row value represents the day of the year

EMPTY1 Empty column

x\_top X-coordinate in pixels of top of Crassostrea gigas shell #1 (increment 0)

**y\_top** Y-coordinate in pixels of top of Crassostrea gigas shell #1 (increment 0), second row value represents the age in days (=0)

EMPTY2 Empty column

**x\_1** X-coordinate in pixels of increment 1

y\_1 Y-coordinate in pixels of increment 1, second row value represents the age in days

EMPTY3 Empty column

x\_2 X-coordinate in pixels of increment 2

y\_2 Y-coordinate in pixels of increment 2, second row value represents the age in days

EMPTY4 Empty column

x\_3 X-coordinate in pixels of increment 3

y\_3 Y-coordinate in pixels of increment 3, second row value represents the age in days

EMPTY5 Empty column

**x\_4** X-coordinate in pixels of increment 4

**y\_4** Y-coordinate in pixels of increment 4, second row value represents the age in days **EMPTY6** Empty column

x\_5 X-coordinate in pixels of increment 5

 $y_5$  Y-coordinate in pixels of increment 5, second row value represents the age in days

- EMPTY7 Empty column
- x\_6 X-coordinate in pixels of increment 6
- y\_6 Y-coordinate in pixels of increment 6, second row value represents the age in days
- EMPTY8 Empty column
- x\_bottom X-coordinate in pixels of bottom of Crassostrea gigas shell #1
- **y\_bottom** Y-coordinate in pixels of bottom of Crassostrea gigas shell #1, second row value represents the age in days (= age of death)

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

01\_phase

Characteristics of phase in XRF map of oyster

## Description

A dataset containing trace element concentrations and RGB colour values of a phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

## Usage

data(01\_phase)

#### Format

A data frame with 5 rows and 30 variables:

**Description** Description of phase

Name Name of phase

- **R** R-value of phase colour
- G G-value of phase colour
- **B** B-value of phase colour

density specific density of different phases

C Concentration of C in phase

- O Concentration of O in phase
- Na Concentration of Na in phase

Mg Concentration of Mg in phase

Al Concentration of Al in phase

- Si Concentration of Si in phase
- **P** Concentration of P in phase
- S Concentration of S in phase

- CI Concentration of Cl in phase
- K Concentration of K in phase
- Ca Concentration of Ca in phase
- Ti Concentration of Ti in phase
- Cr Concentration of Cr in phase
- Mn Concentration of Mn in phase
- Fe Concentration of Fe in phase
- Ni Concentration of Ni in phase
- Cu Concentration of Cu in phase
- Zn Concentration of Zn in phase
- Br Concentration of Br in phase
- **Rb** Concentration of Rb in phase
- Sr Concentration of Sr in phase
- Rh Concentration of Rh in phase
- Ba Concentration of Ba in phase
- Pb Concentration of Pb in phase

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

Oyster\_accumulation Calculate trace element accumulation rates

## Description

Function that combines the concentrations of trace elements per sub-increment with a smoothed record of mass accumulation with time to calculate the rate of accumulation of each element through the lifetime of the bivalve. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_accumulation(el_time, subincr_matrix, npma = 10)
```

#### Arguments

el_time	Matrix of trace element concentrations through time
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment
npma	Integer n-value determining the window size of the moving average smoothing of the mass accumulation record

## Details

A record of mass accumulation of the shell is smoothed using a moving average. This mass accumulation record is multiplied with the records of trace element concentrations per sub-increment to obtain a record of mass accumulation of each trace element through time and a record of cumulative trace element accumulation through time

## Value

Matrices of trace element accumulation per sub-increment and cumulative trace element accumulation

M_el_mat	Matrix of mass accumulation per trace element
M_el_mat_c	Matrix of cumulative mass accumulation per trace element

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

#### References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_el\_time"

## Examples

```
AccL<-Oyster_accumulation(el_time, subincr_matrix6, npma = 10)</pre>
```

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Oyster\_combined\_run Runs the growth and trace element model

## Description

Function that runs the bivalve growth and trace element model from start to finish, combining Step 2-6. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_combined\_run(raw\_data, image\_length, season\_length=250, Xstep=0.1, Tstep=1, Oyster\_height, Oyster\_length, name\_file="Oyster\_growth\_model", phases\_name, image\_name, image\_ext, npma=10, name\_shell)

# Arguments

raw_data	Numeric data frame containing the X- and Y-coordinates digitized in Adobe Illustrator or another image processing software
image_length	Measured maximum length of the area of the cross section that is represented in "raw_data"
season_length	Length (in days) of the growth season of the studied bivalve
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments
Tstep	The step size (dt) in time (days) used to interpolate the existing shell increments
Oyster_height	Measured maximum height of the shell
Oyster_length	Measured maximum length of the shell in anterio-posterior direction
name_file	string indicating the name that should be added to all exported model results
phases_name	String of full name (including extension!) of the CSV file that contains informa- tion about the phases in the map
image_name	String of full name of the BMP that needs to be imported, excluding extension
image_ext	Extention of phase map file ("BMP" or "TIF")
npma	Window size of the moving average used to smooth mass gain record from the bivalve growth model
name_shell	string indicating the name that should be added to all exported model results

# Details

Oyster\_growth\_run and Oyster\_phase\_run, bundling and exporting the model results

# Value

Exports matrices containing oyster growth parameters for each sub-increment as well as matrices containing trace element accumulation rates and concentration changes through the shells life time resulting from the trace element model. All these matrices are also exported as a list containing:

<pre>subincr_matrix</pre>	Revised version of the "incr_matrix" data frame that contains characteristics calculated for every sub-increment
phase_stat	matrix of statistics of trace elements and phases in the total map
el_time	Matrix of trace element concentrations through time
M_el_mat	Matrix of mass accumulation per trace element
M_el_mat_c	Matrix of cumulative mass accumulation per trace element

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_growth\_run" and "Oyster\_phase\_run"

Oyster\_Convert\_cross\_section

Function that converts XY-data of digitized cross section

## Description

Takes XY data of digitized growth increments in a shell cross section and converts them to a common X-axis with the correct lengths in millimeters. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Oyster\_Convert\_cross\_section

# Usage

```
Oyster_Convert_cross_section(raw_data, image_length, Xstep = 0.1)
```

## Arguments

raw_data	Numeric data frame containing the X- and Y-coordinates digitized in Adobe Illustrator or another image processing software
image_length	Measured maximum length of the area of the cross section that is represented in "raw_data"
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments

# Details

First step in growth modelling: Converting XY data of increments to a common X-axis

# Value

List of two data sets and one value:

cross_section	Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis
year_trace	Digitized cross section of shell increments without addition of top and bottom of the shell to the increment Y-values
lengthfactor	Factor of actual shell length relative to shell length in cross section
incr_matrix	Matrix containing ages and calibrated ages for each shell increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 - A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

Llist<-Oyster\_Convert\_cross\_section(01\_input, image\_length, Xstep=1)</pre>

```
Oyster_ellipse_parameters
```

Function that calculates the parameters of the base ellipse used for bivalve growth modelling

# Description

Calculates the parameters a and b of the ellipse that forms the base of the shell in growth modelling. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_ellipse_parameters(subincr_matrix, IncG, Oyster_height, Oyster_length)
```

## Arguments

subincr_matrix	Data frame that contains characteristics of every sub-increment
IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
Oyster_height	Measured maximum height of the shell
Oyster_length	Measured maximum length of the shell in anterio-posterior direction

## Details

Parameters of the base ellipse of the shell are calculated by calculating the ratio between measured shell height and length and the endpoints of all sub-increments

## Value

subincr\_matrix Updated data frame that contains characteristics of every sub-increment, with ellipse parameters added

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

#### Oyster\_el\_time

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

#### Examples

subincr\_matrix4<-Oyster\_ellipse\_parameters(subincr\_matrix3,IncG,Oyster\_height,Oyster\_height)</pre>

Oyster\_el\_timeCalculate concentrations of trace elements per sub-increment

#### Description

Function that takes the matrix of phase pixels per sub-increment together with the matrix of concentrations per phase to calculate the concentration of each trace element in every sub-increment. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

Oyster\_el\_time(phase\_mat, phases)

## Arguments

phase_mat	Matrix of amounts of pixels of each phase per sub-increment
phases	Matrix containing colour and trace element data of the phases in the XRF phase
	map

#### Details

For every sub-increment, the relative contribution of phases is multiplied with the trace element concentrations of the phases to calculate the average concentration of trace elements in each sub-increment

## Value

Matrix of trace element concentrations per sub-increment

el\_time Matrix of trace element concentrations through time

#### Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_Volumes"

# Examples

el\_time<-Oyster\_el\_time(phase\_mat, 01\_phase)</pre>

Oyster\_Export Function that exports data of the growth model

#### Description

Function that exports the results of the bivalve growth model as tables in the form of XLSX files. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_Export(subincr\_matrix, name\_file)

# Arguments

subincr_matrix	Data frame that contains characteristics of every sub-increment
name_file	String containing the name of the file to be exported

## Details

Results are exported as "<name file>.xlsx?" in the working directory

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

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## Oyster\_growth\_run

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

# See Also

"Oyster\_av\_thickness"

#### Examples

```
## Not run:
    Oyster_Export(subincr_matrix6, "test_export")
```

## End(Not run)

Oyster\_growth\_run Runs the entire growth model

# Description

Function that runs all functions contained in Step 2-4 of the growth model. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_growth_run(LOG=T, raw_data, image_length, season_length=250,
Xstep=0.1, Tstep=1, Oyster_height, Oyster_length,
name_file="Oyster_growth_model")
```

## Arguments

LOG	Boolean parameter specifying if a LOG should be printed detailing the parameters entered into this function
raw_data	Numeric data frame containing the X- and Y-coordinates digitized in Adobe Illustrator or another image processing software

image_length	Measured maximum length of the area of the cross section that is represented in "raw_data"
season_length	Length (in days) of the growth season of the studied bivalve
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments
Tstep	The step size (dt) in time (days) used to interpolate the existing shell increments
Oyster_height	Measured maximum height of the shell
Oyster_length	Measured maximum length of the shell in anterio-posterior direction
name_file	string indicating the name that should be added to all exported model results

## Details

Runs Oyser\_run\_sec2, Oyser\_run\_sec3, Oyser\_run\_sec4 and Oyster\_Export

## Value

Matrix containing all parameters of the shell calculated per sub-increment and CSV file containing this matrix

subincr\_matrix Revised version of the "incr\_matrix" data frame that contains characteristics calculated for every sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

```
## Not run:
GList<-Oyster_growth_run(TRUE, O1_input, image_length, season_length=250,
Xstep=1, Tstep=1, Oyster_height, Oyster_length,name_file="test_export")
```

## End(Not run)

Oyster\_height Med

## Description

A single value containing the measured height in mm of the Crassostrea gigas #1 oyster used as an example in de Winter (2017) GMD.

## Usage

data(Oyster\_height)

## Format

A single value: Height in mm of the Crassostrea gigas #1 shell

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

Oyster\_import\_BMP Function that imports a BMP of an XRF map

## Description

Function that imports a BMP file into R. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_import_BMP(file_name)
```

## Arguments

file\_name String of full name of the BMP that needs to be imported, excluding the extension

# Details

Requires "bmp" package to work

#### Value

BMP "BMP" file representing the BMP image in R session

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Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

Oyster\_import\_phases Function that imports phase data

#### Description

Function that imports a table (in CSV format) containing the specifics of phases that make up the phase XRF map used in the trace element model. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

Oyster\_import\_phases(file\_name)

#### Arguments

file\_name String containing the name of the CSV file to be imported, including its extension

## Details

This function imports a table containing trace element concentration and RGB colour data. Table needs to be of the same format as the example shown in de Winter, N.J., GMD, in review. The amount of phases represented in the table byrows is unlimited)

## Value

phases Matrix containing colour, density and trace element data of the phases in the XRF phase map

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_av\_thickness"

Oyster\_import\_TIF Function that imports a TIF file

## Description

Function that imports an image in TIF or TIFF format of an XRF map. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_import_TIF(file_name)
```

# Arguments

file\_name String of full name of the TIF(F) that needs to be imported, including extension

# Details

Requires "tiff" package to work

## Value

TIF

"TIF" file representing the TIF(F) image in R session

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_av\_thickness"

Oyster\_incr\_area Area between shell increments

## Description

Calculates the area between this shell increment and the previous increment and the cumulative shell cross section area at the moment of deposition of the current increment and adds these to the previously created increment matrix. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_incr\_area(cross\_section, incr\_matrix)

## Arguments

cross_section	Digitized cross section of the shell with shell top, bottom and growth increments
	relative to a common X-axis
incr_matrix	Matrix containing ages and calibrated ages for each shell increment

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#### Details

Areas between shell increments are calculated by iterating through increments in X-direction (dx) and adding differences in Y-values between increments

## Value

incr\_matrix Matrix containing ages and calibrated ages for each shell increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

incr\_matrix1<-Oyster\_incr\_area(cross\_section, incr\_matrix0)</pre>

Oyster\_incr\_cross\_section

Formula that interpolates shell increments

## Description

Formula that takes the coordinates of digitized shell increments and interpolates a number of subincrements between them to increase the time resolution of the growth model. The number of interpolated shell increments as well as the relative thickness of these increments is determined by a sinusoidal seasonal model that simulates seasonal variations in shell growth rate. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_incr_cross_section(incr_matrix, cross_section, season_length,
    Tstep=1, Xstep=0.1)
```

## Arguments

incr_matrix	Matrix listing characteristics of each digitized increment
cross_section	Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis
season_length	Length (in days) of the growth season of the studied bivalve
Tstep	The step size (dt) in time (days) used to interpolate the existing shell increments
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments

# Details

Sub-increments are reconstructed by interpolating Y-values between the digitized shell increments

# Value

List of two data frames:

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
<pre>subincr_matrix</pre>	Revised version of the "incr_matrix" data frame that contains characteristics
	(sub-increment number, X-value of start of increment) recalculated for every
	sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

#### References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

Lsub<-Oyster\_incr\_cross\_section(incr\_matrix3, cross\_section, season\_length=250, Tstep=1, Xstep=1) Oyster\_length

## Description

A single value containing the measured length (in anterio-posterior direction) in mm of the Crassostrea gigas #1 oyster used as an example in de Winter (2017) GMD.

#### Usage

data(Oyster\_length)

## Format

A single value:

Lenght in mm of the Crassostrea gigas #1 shell

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

Oyster\_Mass\_gain Formula that calculates mass increase of bivalve shell with time

## Description

Formula that takes the modelled volume of a bivalve shell by sub-increment and calculates mass increase using variable shell density. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_Mass\_gain(subincr\_matrix, phase\_mat, phases)

## Arguments

<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment
phase_mat	Matrix of amounts of pixels of each phase per sub-increment
phases	Matrix containing colour, density and trace element data of the phases in the XRF phase map

## Details

Calculates mass gain from modelled changes in volume based on the shell density

#### Value

subincr\_matrix Updated data frame that contains characteristics of every sub-increment with modelled shell mass calculations added to the matrix

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

## Examples

subincr\_matrix6<-Oyster\_Mass\_gain(subincr\_matrix5, phase\_mat, 01\_phase)</pre>

Oyster\_phase\_export Export results of trace element model

## Description

A function that takes all the matrices with results of the trace element model and exports them as XLSX files. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_phase_export(phase_stat, el_time, M_el_mat, M_el_mat_c, name_shell)
```

## Arguments

phase_stat	matrix of statistics of trace elements and phases in the total map
el_time	Matrix of trace element concentrations through time
M_el_mat	Matrix of mass accumulation per trace element
M_el_mat_c	Matrix of cumulative mass accumulation per trace element
name_shell	Name of the shell used in the model to be incorporated into the file names

## Details

All matrices fed to the function are exported as XLSX files in the working directory using the " write.xlsx" function of the "xlsx" package

## Value

XLSX files of all result matrices of the trace element model

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

#### References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_Export"

#### Examples

```
## Not run:
    Oyster_phase_export(phase_stat, el_time, M_el_mat, M_el_mat_c, "test")
```

## End(Not run)

Oyster\_phase\_matrix\_BMP

Function that calculates phase matrix

#### Description

Function that calculates a matrix of phase numbers for every pixel in the imported BMP file. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_phase\_matrix\_BMP(BMP, phases)

## Arguments

BMP	"BMP" file representing the BMP image in R session
phases	Matrix containing colour, density and trace element data of the phases in the XRF phase map

## Details

This function compares the colour data from the "BMP" object with colour codes of phases in "phases" table to assign a phase to every pixel in the BMP

## Value

phasemat matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

## Examples

```
## Not run:
    phasemat<-Oyster_phase_matrix_BMP(BMP, 01_phase)</pre>
```

## End(Not run)

Oyster\_phase\_matrix\_TIF

Function that calculates phase matrix

#### Description

Function that calculates a matrix of phase numbers for every pixel in the imported TIF file. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

Oyster\_phase\_matrix\_TIF(TIF, phases)

#### Arguments

TIF	"TIF" file representing the TIF(F) image in R session
phases	Matrix containing colour and trace element data of the phases in the XRF phase
	map

## Details

This function compares the colour data from the "TIF" object with colour codes of phases in "phases" table to assign a phase to every pixel in the TIF(F)

## Value

phasemat matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_av\_thickness"

## Examples

```
## Not run:
    phasemat<-Oyster_phase_matrix_TIF(TIF, 01_phase)</pre>
```

## End(Not run)

Oyster\_phase\_run Runs the entire trace element model

## Description

Function that runs all functions contained in Step 5 and 6 of the trace element model. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_phase_run(LOG=T, phases_name, image_name, image_ext, IncG,
    pixelsize, subincr_matrix, npma=10, name_shell, name_file)
```

# Arguments

LOG	Boolean parameter specifying if a LOG should be printed detailing the parameters entered into this function
phases_name	String of full name (including extension!) of the CSV file that contains informa- tion about the phases in the map
image_name	String of full name of the BMP that needs to be imported, excluding extension
image_ext	Extention of phase map file ("BMP" or "TIF")
IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
pixelsize	Size of pixels in phase map in micrometeres

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<pre>subincr_matrix</pre>	Revised version of the "yearly_matrix" data frame that contains characteristics calculated for every sub-increment
npma	Window size of the moving average used to smooth mass gain record from the bivalve growth model
name_shell	string indicating the name that should be added to all exported model results
name_file	string indicating the name of the exported results file

## Details

Runs Oyser\_run\_sec5, Oyser\_run\_sec6 and Oyster\_phase\_export

# Value

XLSX files of all result matrices of the trace element model as well as a list containing these matrices:

phase_stat	matrix of statistics of trace elements and phases in the total map
el_time	Matrix of trace element concentrations through time
M_el_mat	Matrix of mass accumulation per trace element
M_el_mat_c	Matrix of cumulative mass accumulation per trace element

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

Oyster\_phase\_stats Function that exports phase statistics

#### Description

Function that searches through the matrix of phases per pixel and exports the statistics of representation of different phases in the map as well as the bulk composition of pixels in the map. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_phase\_stats(phasemat, phases)

## Arguments

phasemat	matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel
phases	Matrix containing colour and trace element data of the phases in the XRF phase
	map

## Details

Phase statistics are calculated by looping through the matrix of phases created from the XRF phase map and comparing with the "phases" statistics table

#### Value

phase\_stat matrix of statistics of trace elements and phases in the total map

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.
Oyster\_plot\_cross\_section

## See Also

"Oyster\_phase\_matrix\_BMP"

#### Examples

phase\_stat<-Oyster\_phase\_stats(phasemat, 01\_phase)</pre>

Oyster\_plot\_cross\_section

Plot the converted shell cross section

#### Description

Simple function that returns a plot of the shell cross section after it has been converted to a common X-axis. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

# Usage

Oyster\_plot\_cross\_section(cross\_section)

#### Arguments

cross\_section Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis

# Details

Plotting of digitized cross section after first modelling step to verify the correct digitization of the shell increments

## Value

Opens a new plotting window to plot the shell cross section based on its X- and Y-coordinates

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

Oyster\_plot\_cross\_section(cross\_section)

Oyster\_plot\_incr\_CS Plot the result of interpolation of sub-increments

## Description

Formula that plots the result of the interpolation of digitized shell growth increments to reconstruct sub-increments to provide a check on the progress of the model. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

# Usage

Oyster\_plot\_incr\_CS(IncG, incr\_matrix, Tstep)

## Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
incr_matrix	Matrix listing characteristics of each digitized increment
Tstep	The step size (dt) in time (days) used to interpolate the existing shell increments

#### Details

In order to prevent overcrowding the plot area and slowing the plotting process, only original shell increments and sub-increments halfway between original increments are plotted. Sub-increments are colored blue

## Value

No data is exported, but a plot showing interpolated sub-increments is given in a separate window.

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

#### Oyster\_plot\_incr\_fill

## Source

```
GitHub
Manuscript
Supplementary data
Author website
```

#### References

de Winter, N. J.: ShellTrace v1.0 - A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

Oyster\_plot\_incr\_CS(IncG,incr\_matrix3,Tstep=1)

Oyster\_plot\_incr\_fill Plot the result of interpolation of sub-increments with a coloured area plot

#### Description

Formula that plots the result of the interpolation of digitized shell growth increments to reconstruct sub-increments to provide a check on the progress of the model. Areas between sub-increments are coloured in direction of growth using the heat colour palette. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_plot_incr_fill(IncG)
```

#### Arguments

IncG

Matrix of X- and Y-coordinates of all interpolated sub-increments

#### **Details**

Areas between sub-increments are represented by coloured polygons, while digitized increments are plotted using black lines. High numbers of interpolated sub-increments can cause plotting to become slow

## Value

No data is exported, but a coloured plot showing interpolated sub-increments is given in a separate window.

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 - A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

# Examples

```
Oyster_plot_incr_fill(IncG)
```

Oyster_run_sec2	Runs complete Step 2 of the growth model
	r = r = r = r

# Description

Function that combines all functions in Step 2 of the bivalve growth model and runs them consecutively given the right input. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

# Usage

```
Oyster_run_sec2(raw_data, image_length, Xstep)
```

# Arguments

raw_data	Numeric data frame containing the X- and Y-coordinates digitized in Adobe Illustrator or another image processing software
image_length	Measured maximum length of the area of the cross section that is represented in raw_data
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments

# Details

This function runs the functions Oyster\_Convert\_cross\_section, Oyster\_plot\_cross\_section, Oyster\_incr\_area, Oyster\_Shell\_thickness and Oyster\_Shell\_height consecutively

# Value

List of three items:

cross_section	Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis
incr_matrix	Matrix listing characteristics of each digitized increment
lengthfactor	Factor of actual shell length relative to shell length in cross section, used to constrain pixelsize in phase map

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

# Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

List2<-Oyster\_run\_sec2(01\_input, image\_length, Xstep=1)</pre>

Oyster\_run\_sec3

#### Description

Function that combines all functions in Step 3 of the bivalve growth model and runs them consecutively given the right input. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

# Usage

```
Oyster_run_sec3(cross_section, incr_matrix, season_length=250, Xstep=0.1,
Tstep=1, Oyster_height, Oyster_length)
```

## Arguments

cross_section	Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis
incr_matrix	Matrix listing characteristics of each digitized increment
season_length	Length (in days) of the growth season of the studied bivalve
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments
Tstep	The step size (dt) in time (days) used to interpolate the existing shell increments
Oyster_height	Measured maximum height of the shell
Oyster_length	Measured maximum length of the shell in anterio-posterior direction

# Details

This function runs the functions Oyster\_Increment\_cross\_section, Oyster\_plot\_Inc\_CS, Oyster\_Inc\_fill, Oyster\_subincr\_area, Oyster\_subincr\_shell\_height, Oyster\_subincr\_av\_thickness and Oyster\_ellipse\_parameters consecutively

## Value

List of two items:

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
subincr_matrix	Revised version of the "yearly_matrix" data frame that contains characteristics (sub-increment number, X-value of start of increment) recalculated for every sub-increment

#### Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

# Oyster\_run\_sec4

# Source

```
GitHub
Manuscript
Supplementary data
Author website
```

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

```
List3<-Oyster_run_sec3(cross_section, incr_matrix3, season_length=250, Xstep=1,
Tstep=1, Oyster_height, Oyster_length)
```

Ovster_run_sec4 Runs complete	e Step 4 of the growth model
-------------------------------	------------------------------

# Description

Function that combines all functions in Step 4 of the bivalve growth model and runs them consecutively given the right input. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

Oyster\_run\_sec4(IncG, subincr\_matrix, Xstep = 0.1)

#### Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
<pre>subincr_matrix</pre>	Revised version of the "yearly_matrix" data frame that contains characteristics calculated for every sub-increment
Xstep	The step size (dx) in X-direction used to interpolate coordinates of shell incre- ments

## Details

This function runs the functions Oyster\_Z\_matrices and Oyster\_Volumes consecutively

#### Value

A list of two items:

<pre>subincr_matrix</pre>	Revised version of the "incr_matrix" data frame that contains characteristics
	calculated for every sub-increment
IncGAnet	Matrix of areas of cross sections in YZ-directions sorted by X-values and by
	sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### Examples

```
## Not run:
List4<-Oyster_run_sec4(IncG, subincr_matrix4, Xstep = 1)
## End(Not run)
```

Oyster\_run\_sec5 Runs complete Step 5 of the trace element model

## Description

Function that combines all functions in Step 5 of the bivalve trace element model and runs them consecutively given the right input. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_run_sec5(phases_name, image_name, image_ext)
```

#### Arguments

phases_name	String of full name (including extension!) of the CSV file that contains informa- tion about the phases in the map
image_name	String of full name of the BMP that needs to be imported, excluding extension
image_ext	Extention of phase map file ("BMP" or "TIF")

# Oyster\_run\_sec6

## Details

This function runs the functions Oyster\_import\_phases, Oyster\_phase\_matrix\_BMP, Oyster\_phase\_matrix\_TIF and Oyster\_phase\_stat consecutively

#### Value

List of two items:

phasemat	matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel
phase_stat	matrix of statistics of trace elements and phases in the total map
phases	Matrix containing colour, density and trace element data of the phases in the XRF phase map

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

Oyster\_run\_sec6Runs complete Step 6 of the trace element model

# Description

Function that combines all functions in Step 6 of the bivalve trace element model and runs them consecutively given the right input. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

```
Oyster_run_sec6(phasemat, IncG, pixelsize, phases, subincr_matrix, npma,
    name_file)
```

## Arguments

phasemat	matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel
IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
pixelsize	size of pixels in the phase map in micrometer
phases	Matrix containing colour and trace element data of the phases in the XRF phase map
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment
npma	Integer n-value determining the window size of the moving average smoothing of the mass accumulation record
name_file	string indicating the name of the exported results file

# Details

This function runs the functions Oyster\_subincr\_phases, Oyster\_Mass\_gain Oyster\_el\_time and Oyster\_accumulation consecutively

# Value

List of three items:

el_time	Matrix of trace element concentrations through time
M_el_mat	Matrix of mass accumulation per trace element
M_el_mat_c	Matrix of cumulative mass accumulation per trace element
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

# Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

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# Oyster\_Shell\_height

## Examples

```
## Not run:
List6<-Oyster_run_sec6(phasemat, IncG, pixelsize, O1_phase, subincr_matrix5, npma=10,
    "test_export")
```

## End(Not run)

Oyster\_Shell\_height Formula that calculates shell height through time

# Description

Formula that calculates shell height at the moment of deposition of each shell increment from X- and Y-coordinates of the shell increments and adds the result to the matrix of increment characteristics. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

```
Oyster_Shell_height(cross_section, incr_matrix)
```

# Arguments

incr_matrix	Matrix listing characteristics of each digitized increment
cross_section	Digitized cross section of the shell with shell top, bottom and growth increments relative to a common X-axis

#### Details

Shell height is calculated via the Pythagorean Theorem using the X- and Y-coordinates of both ends of the shell increment with extreme X-values

#### Value

incr\_matrix Updated matrix listing characteristics of each digitized increment, shell height values as well as the coordinates of both ends of the shell increments are added

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

# Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

incr\_matrix3<-Oyster\_Shell\_height(cross\_section, incr\_matrix2)</pre>

Oyster\_Shell\_thickness

Formula that calculates average shell thickness through time

## Description

Formula that calculates average shell thickness at the moment of deposition of each shell increment from X- and Y-coordinates of the shell increments and adds the result to the matrix of increment characteristics. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

#### Usage

Oyster\_Shell\_thickness(cross\_section, incr\_matrix)

## Arguments

incr_matrix	Matrix listing characteristics of each digitized increment
cross_section	Digitized cross section of the shell with shell top, bottom and growth increments
	relative to a common X-axis

## Details

Shell thickness is calculated as the average difference in Y-values between the shell increment and the top of the shell (Increment 0)

## Value

incr\_matrix Updated matrix listing characteristics of each digitized increment, shell thickness values are added

A plot of the change in shell thickness with shell age based on the digitized growth increments is produced in a new window

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# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### Examples

incr\_matrix2<-Oyster\_Shell\_thickness(cross\_section, incr\_matrix1)</pre>

Oyster\_subincr\_area Formula that calculates area between sub-increments

## Description

Formula that calculates cross section area between each sub-increment and the previous sub-increment. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

Oyster\_subincr\_area(IncG, subincr\_matrix, Xstep)

## Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment
Xstep	Step value in X-direction for the interpolation of sub-increments

#### Details

Areas between sub-increments are calculated by averaging the difference in Y-values between sub-increments and multiplying them with the step in X-values (dx)

#### Value

subincr\_matrix Revised version of the "incr\_matrix" data frame that contains cross section area recalculated for every sub-increment

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_Shell\_length"

## Examples

subincr\_matrix1<-Oyster\_subincr\_area(IncG, subincr\_matrix0, Xstep=1)</pre>

Oyster\_subincr\_av\_thickness

Formula that calculates average shell thickness through time

## Description

Formula that calculates average shell thickness at the moment of deposition of each shell subincrement from cross section area and shell length and adds the result to the matrix of increment characteristics. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

# Usage

Oyster\_subincr\_av\_thickness(subincr\_matrix)

## Arguments

subincr\_matrix Data frame that contains characteristics of every sub-increment

# Details

Shell thickness is calculated as the ratio between cross section area and shell length (Increment 0)

## Value

subincr\_matrix Revised version of the "incr\_matrix" data frame that contains average shell thickness recalculated for every sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

## Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

# See Also

"Oyster\_av\_thickness"

## Examples

subincr\_matrix3<-Oyster\_subincr\_av\_thickness(subincr\_matrix2)</pre>

Oyster\_subincr\_av\_thickness\_X

Formula that calculates average shell thickness through time

#### Description

Formula that calculates average shell thickness at the moment of deposition of each shell subincrement from X- and Y-coordinates of the shell increments and adds the result to the matrix of increment characteristics. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_subincr_av_thickness_X(IncG, subincr_matrix)
```

#### Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment

# Details

Shell thickness is calculated as the average difference in Y-values between the shell sub-increment and the top of the shell (Increment 0)

# Value

subincr\_matrix Revised version of the "incr\_matrix" data frame that contains average shell thickness recalculated for every sub-increment

#### Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

#### Examples

```
subincr_matrix3<-Oyster_subincr_av_thickness_X(IncG, subincr_matrix2)</pre>
```

Oyster\_subincr\_phases Calculates proportion of phases in each sub-increment

## Description

Function that takes the matrix of sub-increment positions and the matrix of phases and calculates the amount of pixels of each phase that is contained in each sub-increment based on pixelsize and phase characteristics. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_subincr_phases(IncG, phasemat, pixelsize, phases)
```

#### Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
phasemat	matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel
pixelsize	size of pixels in the phase map in millimeter
phases	Matrix containing colour and trace element data of the phases in the XRF phase
	map

#### Details

For every sub-increment, all pixels that cover area in the sub-increment are identified based on the pixel size of the phase map and the X- and Y-positions of the sub-increments. The amount of pixels of each phase in the sub-increment is saved in a new matrix of phases per sub-increment

## Value

A matrix of the amount of pixels for each phase found in every sub-increment

phase\_mat Matrix of amounts of pixels of each phase per sub-increment

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

# Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_Suby\_av\_thickness"

# Examples

```
## Not run:
    phase_mat<-Oyster_subincr_phases(IncG, phasemat, pixelsize, 01_phase)</pre>
```

## End(Not run)

```
Oyster_subincr_shell_height
```

A fomula to calculate shell height per sub-increment

# Description

Formula that calculates shell height at the time of deposition of each sub-increment. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_subincr_shell_height(subincr_matrix, IncG, Xstep)
```

# Arguments

subincr_matrix	Data frame that contains characteristics of every sub-increment
IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
Xstep	Step value in X-direction for the interpolation of sub-increments

## Details

Shell height is calculated via the Pythagorean Theorem using the X- and Y-coordinates of both ends of the shell sub-increment with extreme X-values

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# Oyster\_Volumes

# Value

subincr\_matrix Revised version of the "incr\_matrix" data frame that contains shell height recalculated for every sub-increment

#### Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

#### References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

# See Also

"Oyster\_Shell\_height"

# Examples

subincr\_matrix2<-Oyster\_subincr\_shell\_height(subincr\_matrix1,IncG,Xstep=1)</pre>

Oyster\_Volumes Formula that calculates volume of the shell through time

#### Description

Formula that calculates the volume of the bivalve shell during the time of deposition of each subincrement. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

```
Oyster_Volumes(subincr_matrix, Z_mat, IncG, Xstep = 0.1)
```

## Arguments

<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment
Z_mat	Matrix of Z-values for each X-value and each sub-increment
IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
Xstep	Step value in X-direction for the interpolation of sub-increments

# Details

Volume is calculated for each sub-increment and each X-value based on cross sections perpendicular to the XY-plane. Area of the shell in this cross section is calculated by constructing a circle section through the intercept with the base ellipse and the top of the shell sub-increment. See paper de Winter, GMD (in review) for details and illustrations

#### Value

A list of two data frames:

subincr_matrix	Updated data frame that contains characteristics of every sub-increment with modelled shell volumes added to the matrix
IncGAnet	Matrix of areas of cross sections in YZ-directions sorted by X-values and by sub-increment

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

## Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

"Oyster\_av\_thickness"

# Oyster\_Z\_matrices

# Examples

```
## Not run:
    diagL<-Oyster_Volumes(subincr_matrix4, Z_mat, IncG, Xstep = 1)</pre>
```

## End(Not run)

Oyster\_Z\_matrices Function that calculates matrices of Z-values for all sub-increments and all X-values

## Description

Function that calculates Z-values that form the edge of the shell in terms of distance from the X-axis in direction of the width of the shell. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

```
Oyster_Z_matrices(IncG, subincr_matrix)
```

# Arguments

IncG	Matrix of X- and Y-coordinates of all interpolated sub-increments
<pre>subincr_matrix</pre>	Data frame that contains characteristics of every sub-increment

# Details

Z-values are calculated using the standard formulae of an ellipse, the parameters calculated in "Oys-ter\_Oval\_parameters" and the X-coordinates of each sub-increment

# Value

Z-mat Matrix of Z-values for each X-value and each sub-increment

# Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

# Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

## References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

#### See Also

"Oyster\_av\_thickness"

# Examples

Z\_mat<-Oyster\_Z\_matrices(IncG, subincr\_matrix4)</pre>

phasemat

Matrix of phases names for each pixel in the phase map

# Description

A dataset containing names of phases for every pixel in the phase map measured on a cross section through the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

#### Usage

data(phasemat)

#### Format

A large data frame with 2258 rows and 2383 variables:

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

phase\_mat

Matrix listing the amount of pixels of each phase in every subincrement

## Description

A dataset containing the amounts of pixels of each phase in the phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017) represented in every subincrement.

#### Usage

data(phase\_mat)

#### phase\_stat

## Format

A data frame with 4 rows and 1291 variables:

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

phase\_stat

Statistics of elemental concentrations in XRF map of oyster

## Description

A dataset containing trace element concentrations and fractions of a phase map of the XRF mapped surface of the Crassostrea gigas #1 oyster used as an example in de Winter (2017)

## Usage

data(phase\_stat)

# Format

A data frame with 5 rows and 27 variables:

Names Names of phases

pixels Amount of pixels representing the phase

fraction Fraction of map surface represented by phase

C Concentration of C in phase

**O** Concentration of O in phase

Na Concentration of Na in phase

Mg Concentration of Mg in phase

Al Concentration of Al in phase

Si Concentration of Si in phase

**P** Concentration of P in phase

S Concentration of S in phase

Cl Concentration of Cl in phase

K Concentration of K in phase

Ca Concentration of Ca in phase

Ti Concentration of Ti in phase

Cr Concentration of Cr in phase

Mn Concentration of Mn in phase

Fe Concentration of Fe in phase

- Ni Concentration of Ni in phase
- Cu Concentration of Cu in phase
- Zn Concentration of Zn in phase
- Br Concentration of Br in phase
- **Rb** Concentration of Rb in phase
- Sr Concentration of Sr in phase
- Rh Concentration of Rh in phase
- Ba Concentration of Ba in phase
- **Pb** Concentration of Pb in phase

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

pixelsize

Size of pixels in phase map in mm

# Description

A single value of the amount of mm contained in one pixel rounded up to the nearest micrometer.

#### Usage

data(pixelsize)

#### Format

A single value:

Length in mm of one pixel in the digitized shell cross section rounded up to the nearest micrometer

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

# Description

Performs a moving average smoothing on a data series. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Usage

pma(x, i, n)

## Arguments

x	A numeric data frame containing the data set to be smoothed, X-values should be in the first column
i	The index of the column that contains the Y-values
n	Integer N-value determining the window size of the moving average smoothing

# Value

A numeric data frame containing three columns: One with X-values, one with Y-values and one with smoothed Y-values

## Note

Please cite Geoscientific Model Development paper dealing with the ShellTrace model

#### Author(s)

Niels J. de Winter

#### Source

GitHub Manuscript Supplementary data Author website

# References

de Winter, N. J.: ShellTrace v1.0 ? A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## Examples

```
Nile<-as.data.frame(Nile)
Nile<-cbind(rownames(Nile),Nile)
Nile_5pma<-pma(Nile,2,5)</pre>
```

ShellTrace

ShellTrace: Growth and trace element uptake modelling in bivalve shells

#### Description

This package contains formulae used to model the growth and development of bivalve shells based on digitized coordinated of shell increments in a longitudinal cross section thorugh the shell. The growth model is combined with XRF mapping results of the same cross section and a seasonal growth rate model to model trace element concentrations and uptake rates into the bivalve shell. de Winter, N. J. (2017) <doi:10.5194/gmd-2017-137>

## Details

Formulae in this package form the several steps of the model, and are not meant to be used individually. The order and application of these functions is outlined in the publication in Geoscientific Model Development that bears the name of the model (de Winter, in review)

## Author(s)

Niels J. de Winter Maintainer: Niels J. de Winter

## References

de Winter, N. J.: ShellTrace v1.0 - A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-137, in review, 2017.

## See Also

GitHub Manuscript Supplementary data Author website

# Examples

print("de Winter, N. J.: ShellTrace v1.0 - A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas), Geosci. Model Dev. Discuss., in review, 2017.")

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subincr\_matrix0

## Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

```
data(subincr_matrix0)
```

#### Format

A data frame with 1291 rows and 3 variables:

Age age (in days) of the subincrement

**p1xs** X-value of the first (leftmost) point in the subincrement

p2xs X-value of the last (rightmost) point in the subincrement

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix1 Matrix containing data calculated for each growth band.

# Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

```
data(subincr_matrix1)
```

#### Format

A data frame with 1291 rows and 5 variables:

Age age (in days) of the subincrement

**p1xs** X-value of the first (leftmost) point in the subincrement

p2xs X-value of the last (rightmost) point in the subincrement

areaY Area between subsequent subincrements

areaC Area between subincrement and top of shell

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix2 Matrix containing data calculated for each growth band.

# Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

data(subincr\_matrix2)

#### Format

A data frame with 1291 rows and 10 variables:

Age age (in days) of the subincrement

plxs X-value of the first (leftmost) point in the subincrement

**p2xs** X-value of the last (rightmost) point in the subincrement

areaY Area between subsequent subincrements

areaC Area between subincrement and top of shell

**p1y** Y-value of the first (leftmost) point in the subincrement

p2y Y-value of the last (rightmost) point in the subincrement

shell\_height Height of shell during deposition of the subincrement

firstl Row number in IncG of first (leftmost) data point belonging to the subincrement

lastl Row number in IncG of last (rightmost) data point belonging to the subincrement

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix3

#### Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

#### Usage

```
data(subincr_matrix3)
```

#### Format

A data frame with 1291 rows and 11 variables:

Age age (in days) of the subincrement
p1xs X-value of the first (leftmost) point in the subincrement
p2xs X-value of the last (rightmost) point in the subincrement
areaY Area between subsequent subincrements
areaC Area between subincrement and top of shell
p1y Y-value of the first (leftmost) point in the subincrement
p2y Y-value of the last (rightmost) point in the subincrement
shell\_height Height of shell during deposition of the subincrement
firstl Row number in IncG of first (leftmost) data point belonging to the subincrement
av\_thickness Average thickness during deposition of the subincrement

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix4 Matrix containing data calculated for each growth band.

#### Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

```
data(subincr_matrix4)
```

## Format

A data frame with 1291 rows and 15 variables:

Age age (in days) of the subincrement

**p1xs** X-value of the first (leftmost) point in the subincrement

**p2xs** X-value of the last (rightmost) point in the subincrement

areaY Area between subsequent subincrements

areaC Area between subincrement and top of shell

ply Y-value of the first (leftmost) point in the subincrement

**p2y** Y-value of the last (rightmost) point in the subincrement

shell\_height Height of shell during deposition of the subincrement

firstl Row number in IncG of first (leftmost) data point belonging to the subincrement

last Row number in IncG of last (rightmost) data point belonging to the subincrement

av\_thickness Average thickness during deposition of the subincrement

- W\_ellipse Length of the short axis of the base ellipse of the oyster during deposition of the subincrement
- L\_ellipse\_acc Length of the long axis of the base ellipse of the oyster during deposition of the subincrement projected on the X-axis
- a\_ellipse Half the length of the long axis of the base ellipse of the oyster during deposition of the subincrement
- **b\_ellipse** Half the length of the short axis of the base ellipse of the oyster during deposition of the subincrement

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix5 *Matrix containing data calculated for each growth band.* 

## Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

```
data(subincr_matrix5)
```

#### Format

A data frame with 1291 rows and 17 variables:

Age age (in days) of the subincrement

plxs X-value of the first (leftmost) point in the subincrement

p2xs X-value of the last (rightmost) point in the subincrement

areaY Area between subsequent subincrements

areaC Area between subincrement and top of shell

**p1y** Y-value of the first (leftmost) point in the subincrement

**p2y** Y-value of the last (rightmost) point in the subincrement

shell\_height Height of shell during deposition of the subincrement

firstl Row number in IncG of first (leftmost) data point belonging to the subincrement

last Row number in IncG of last (rightmost) data point belonging to the subincrement

av\_thickness Average thickness during deposition of the subincrement

- W\_ellipse Length of the short axis of the base ellipse of the oyster during deposition of the subincrement
- L\_ellipse\_acc Length of the long axis of the base ellipse of the oyster during deposition of the subincrement projected on the X-axis
- **a\_ellipse** Half the length of the long axis of the base ellipse of the oyster during deposition of the subincrement
- **b\_ellipse** Half the length of the short axis of the base ellipse of the oyster during deposition of the subincrement
- VolI Volume between subsequent subincrements
- VolC Volume between subincrement and top of shell

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

subincr\_matrix6 Matrix containing data calculated for each growth band.

# Description

A dataset containing specific parameters calculated for all interpolated subincrements from the Crassostrea gigas #1 oyster used as an example in de Winter (2017) sorted per increment.

```
data(subincr_matrix6)
```

#### Format

A data frame with 1291 rows and 20 variables:

Age age (in days) of the subincrement

**p1xs** X-value of the first (leftmost) point in the subincrement

p2xs X-value of the last (rightmost) point in the subincrement

areaY Area between subsequent subincrements

areaC Area between subincrement and top of shell

ply Y-value of the first (leftmost) point in the subincrement

**p2y** Y-value of the last (rightmost) point in the subincrement

shell\_height Height of shell during deposition of the subincrement

firstl Row number in IncG of first (leftmost) data point belonging to the subincrement

last Row number in IncG of last (rightmost) data point belonging to the subincrement

- av\_thickness Average thickness during deposition of the subincrement
- W\_ellipse Length of the short axis of the base ellipse of the oyster during deposition of the subincrement
- L\_ellipse\_acc Length of the long axis of the base ellipse of the oyster during deposition of the subincrement projected on the X-axis
- **a\_ellipse** Half the length of the long axis of the base ellipse of the oyster during deposition of the subincrement
- **b\_ellipse** Half the length of the short axis of the base ellipse of the oyster during deposition of the subincrement
- **VolI** Volume between subsequent subincrements

VolC Volume between subincrement and top of shell

Weight I Mass of shell material between subsequent subincrements

Growth\_rate Mass of shell material accumulated per day

WeightC Mass of shell material between subincrement and top of shell

#### Source

https://doi.org/10.5194/gmd-2017-137-supplement

## Description

An image of the microXRF phase map of the cross section used for this model from the Crassostre gigas #1 oyster used as an example in de Winter (2017)

## Usage

data(TIF)

# Format

A TIF image imported into R as a large data array

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

Z\_mat

*Z*-values describing the base ellipse of the oyster

# Description

A dataset containing Z-coordinates of the base ellipse calculated for all subincrements in the Crassostrea gigas #1 oyster used as an example in de Winter (2017). A Xstep of 0.1, a Tstep of 1 and a growth season of 250 days are used.

#### Usage

data(Z\_mat)

#### Format

A large data frame with 101 rows and 1291 variables:

## Source

https://doi.org/10.5194/gmd-2017-137-supplement

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