

Package ‘shelltrace’

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Type Package

Title Bivalve Growth and Trace Element Accumulation Model

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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 equally-named

Geoscientific Model Development paper (de Winter, 2017, <[doi:10.5194/gmd-2017-137](https://doi.org/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 calcu-

late 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 mod-

elling are combined with the trace element mapping

results to trace the incorporation of trace elements into the bivalve shell. Results of various mod-

elling parameters can be exported in

the form of XLSX files.

License GPL-3

LazyData true

URL <https://github.com/nielsjdewinter/ShellTrace>,
<https://doi.org/10.5194/gmd-2017-137-supplement>,
<http://nidewint.wixsite.com/nielsdewinter>

BugReports <https://github.com/nielsjdewinter/ShellTrace/issues>

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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 Crassostrea 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	<i>Digitized growth increments in cross section of modern oyster rescaled to the same X-axis.</i>
---------------	---

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	<i>Matrix listing the concentrations of elements in every subincrement</i>
---------	--

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)
```

Format

A data frame with 24 rows and 1291 variables:

Source

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

image_length	<i>Length (in mm) of the digitized phase map image.</i>
--------------	---

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	<i>Interpolated subincrements in cross section of modern oyster rescaled to the same X-axis.</i>
------	--

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	<i>Matrix containing data calculated for each growth band.</i>
--------------	--

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	<i>Matrix containing data calculated for each growth band.</i>
--------------	--

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

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)
```

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

p1y 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>

M_el_mat

*Matrix of modelled mass accumulation rates per trace element***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	<i>Matrix of modelled cumulative mass accumulation rates per trace element</i>
------------	--

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

Source

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

O1_input	<i>Digitized growth increments in cross section of modern oyster.</i>
----------	---

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(O1_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>

O1_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(O1_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

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>

Oyster_accumulation	<i>Calculate trace element accumulation rates</i>
---------------------	---

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

<code>el_time</code>	Matrix of trace element concentrations through time
<code>subincr_matrix</code>	Data frame that contains characteristics of every sub-increment
<code>npma</code>	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)
```

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 increments
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 antero-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 information about the phases in the map
image_name	String of full name of the BMP that needs to be imported, excluding extension
image_ext	Extension 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:

subincr_matrix	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](https://doi.org/10.5194/gmd-2017-137)>

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 increments

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(O1_input, image_length, Xstep=1)
```

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 antero-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](#)

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)
```

Oyster_el_time

Calculate 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](https://doi.org/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)
```

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](https://doi.org/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

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	<i>Runs the entire growth model</i>
-------------------	-------------------------------------

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](https://doi.org/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 increments
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 antero-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, 01_input, image_length, season_length=250,
Xstep=1, Tstep=1, Oyster_height, Oyster_length,name_file="test_export")

## End(Not run)
```

Oyster_height	<i>Measured height of the shell</i>
---------------	-------------------------------------

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	<i>Function that imports a BMP of an XRF map</i>
-------------------	--

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
-----	--

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](https://doi.org/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](https://doi.org/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	<i>Area between shell increments</i>
------------------	--------------------------------------

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](https://doi.org/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

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)
```

Oyster_incr_cross_section

Formula that interpolates shell increments

Description

Formula that takes the coordinates of digitized shell increments and interpolates a number of sub-increments 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](https://doi.org/10.5194/gmd-2017-137)>

Usage

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

Arguments

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

Details

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

Value

List of two data frames:

<code>IncG</code>	Matrix of X- and Y-coordinates of all interpolated sub-increments
<code>subincr_matrix</code>	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	<i>Measured length of the shell</i>
---------------	-------------------------------------

Description

A single value containing the measured length (in antero-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:
Length in mm of the Crassostrea gigas #1 shell

Source

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

Oyster_Mass_gain	<i>Formula that calculates mass increase of bivalve shell with time</i>
------------------	---

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

subincr_matrix	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)
```

Oyster_phase_export	<i>Export results of trace element model</i>
---------------------	--

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](https://doi.org/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)

## 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)

## End(Not run)
```

Oyster_phase_run	<i>Runs the entire trace element model</i>
------------------	--

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](https://doi.org/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 information about the phases in the map
image_name	String of full name of the BMP that needs to be imported, excluding extension
image_ext	Extension 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 micrometers

subincr_matrix	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	<i>Function that exports phase statistics</i>
--------------------	---

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.

See Also

"Oyster_phase_matrix_BMP"

Examples

```
phase_stat<-Oyster_phase_stats(phasemat, 01_phase)
```

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	<i>Plot the result of interpolation of sub-increments</i>
---------------------	---

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](https://doi.org/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

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

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](https://doi.org/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 increments

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:

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

Oyster_run_sec3	<i>Runs complete Step 3 of the growth model</i>
-----------------	---

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 increments
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 antero-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

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)
```

Oyster_run_sec4	<i>Runs complete Step 4 of the growth model</i>
-----------------	---

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](https://doi.org/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
subincr_matrix	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 increments

Details

This function runs the functions `Oyster_Z_matrices` and `Oyster_Volumes` consecutively

Value

A list of two items:

subincr_matrix	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	<i>Runs complete Step 5 of the trace element model</i>
-----------------	--

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](https://doi.org/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 information 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")

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:

<code>phasemat</code>	matrix of phases of each pixel sorted by X- and Y-coordinate of the pixel
<code>phase_stat</code>	matrix of statistics of trace elements and phases in the total map
<code>phases</code>	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_sec6`*Runs 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](https://doi.org/10.5194/gmd-2017-137)>

Usage

```
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
subincr_matrix	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
subincr_matrix	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.

Examples

```
## Not run:  
List6<-Oyster_run_sec6(phasemat, IncG, pixelsize, 01_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)
```

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](https://doi.org/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

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)
```

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](https://doi.org/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
subincr_matrix	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)
```

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 sub-increment 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](https://doi.org/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)
```

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 sub-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_subincr_av_thickness_X(IncG, subincr_matrix)
```

Arguments

IncG Matrix of X- and Y-coordinates of all interpolated sub-increments
subincr_matrix 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)
```

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 pixel size 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)

## 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](https://doi.org/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

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)
```

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 sub-increment. de Winter, N. J. (2017) <[doi:10.5194/gmd-2017-137](https://doi.org/10.5194/gmd-2017-137)>

Usage

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

Arguments

subincr_matrix	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"

Examples

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

Oyster_Z_matrices	<i>Function that calculates matrices of Z-values for all sub-increments and all X-values</i>
-------------------	--

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
subincr_matrix	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 "Oyster_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)
```

phasemat	<i>Matrix of phases names for each pixel in the phase map</i>
----------	---

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	<i>Matrix listing the amount of pixels of each phase in every subincrement</i>
-----------	--

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)
```

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	<i>Size of pixels in phase map in mm</i>
-----------	--

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>

pma

Function to do an n-point moving average

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)
```

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 thorough 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.")
```

subincr_matrix0	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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

Source

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

subincr_matrix2	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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

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

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

lastI 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	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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

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

lastI Row number in IncG of last (rightmost) 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	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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_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
- 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
- firstI** Row number in IncG of first (leftmost) data point belonging to the subincrement
- lastI** 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	<i>Matrix containing data calculated for each growth band.</i>
-----------------	--

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_matrix5)

Format

A data frame with 1291 rows and 17 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

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

lastI 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.

Usage

```
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

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

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

lastI 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

WeightI 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>

TIF*TIF 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 *Crassostrea 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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