Package 'RLumModel'

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```
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Title Solving Ordinary Differential Equations to Understand Luminescence
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Description A collection of functions to simulate luminescence sig-
      nals in quartz and Al2O3 based on published models.
Contact Package Developer Team <developer@model.r-luminescence.de>
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BugReports https://github.com/R-Lum/RLumModel/issues
Depends R (>= 4.0),
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      Luminescence (>= 0.9.18)
Imports deSolve (>= 1.30),
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Collate RLumModel-package.R
      RcppExports.R
      calc_signal.R
      calc concentrations.R
      create DRT.sequence.R
      create_SAR.sequence.R
      extract_pars.R
      model_LuminescenceSignals.R
      read_SEQ2R.R
      set_pars.R
      simulate_CW_OSL.R
      simulate_heating.R
```

simulate_illumination.R
simulate_irradiation.R
simulate_LM_OSL.R
simulate_pause.R
simulate_RF.R
simulate_RF_and_heating.R
simulate_TL.R
translate_sequence.R
trace_ParameterStateEvolution.R

RoxygenNote 7.1.2

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LazyData true

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R topics documented:

	RLumModel-package	
	.set_pars	3
	ExampleData.ModelOutput	5
	model_LuminescenceSignals	6
	read_SEQ2R	14
	trace_ParameterStateEvolution	15
Index		17

RLumModel-package Solving Ordinary Differential Equations to Understand Luminescence

Description

Details

A collection of function to simulate luminescence signals in the mineral quartz based on published models.

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Christoph Schmidt, University of Bayreuth, Germany Sebastian Kreutzer, Geography & Earth Sciences, Aberystwyth University, United Kingdom #' **Project source code repository**

• https://github.com/R-Lum/RLumModel

.set_pars 3

Related package projects

- http://r-luminescence.de
- https://CRAN.r-project.org/package=Luminescence
- https://CRAN.r-project.org/package=RLumShiny

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.set_pars

Set parameters for Different Quartz Luminescence Models

Description

This function provides all necessary model parameters to the calculation of the ODEs.

Usage

```
.set_pars(model)
```

Arguments

mode1

character (**required**): set model to be used. Available models are: "Bailey2001", "Bailey2002", "Bailey2004", "Pagonis2007", "Pagonis2008", "Friedrich2017", "Friedrich2018", "Peng2022". If model is indeed missing, the list of allowed keywords is returned.

Details

The common model parameters are:

N: concentrations of electron/hole traps in cm $^{(-3)}$ E: depth of the electron/hole trap in eV s: frequency factor in s $^{(-1)}$ A: conduction band to electron/hole trap transition probability in s $^{(-1)}$ B: valence band to hole trap transition probability in s $^{(-1)}$ Th: photo-ionisation cross-section in s $^{(-1)}$ E_th: thermal assistance energy in (eV) n: concentrations of electron/hole traps after sample history in cm $^{(-3)}$

Value

This function returns a list with all necessary parameters for the used model. Returns vector of allowed keywords if model is missing.

Function version

0.1.3

4 .set_pars

How to cite

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Note

n are the saved concentrations of the last step of the sample history of the used model. They will be loaded, if simulate_sample_history = FALSE in model_LuminescenceSignals is chosen.

The order of the energy-band-levels is sometimes in an different order than in the original model. This was necessary, because in the simulations the luminescence centre always has to be the last entry in every parameter. Another reason was the clear division between electron traps and hole centres. When a user wants to create his/her own parameter sets he/she only has to take care that the luminescence centre is the last entry in every vector and that the first entries are the electron traps and the last entries the hole centres.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany),

References

Bailey, R.M., 2001. Towards a general kinetic model for optically and thermally stimulated luminescence of quartz. Radiation Measurements 33, 17-45.

Bailey, R.M., 2002. Simulations of variability in the luminescence characteristics of natural quartz and its implications for estimates of absorbed dose. Radiation Protection Dosimetry 100, 33-38.

Bailey, R.M., 2004. Paper I-simulation of dose absorption in quartz over geological timescales and its implications for the precision and accuracy of optical dating. Radiation Measurements 38, 299-310.

Friedrich, J., Pagonis, V., Chen, R., Kreutzer, S., Schmidt, C., 2017: Quartz radiofluorescence: a modelling approach. Journal of Luminescence 186, 318-325.

Pagonis, V., Chen, R., Wintle, A.G., 2007. Modelling thermal transfer in optically stimulated luminescence of quartz. Journal of Physics D: Applied Physics 40, 998-1006.

Pagonis, V., Wintle, A.G., Chen, R., Wang, X.L., 2008. A theoretical model for a new dating protocol for quartz based on thermally transferred OSL (TT-OSL). Radiation Measurements 43, 704-708.

Peng, J., Wang, X., Adamiec, G., 2022. The build-up of the laboratory-generated dose-response curve and underestimation of equivalent dose for quartz OSL in the high dose region: A critical modelling study. Quaternary Geochronology 67, 101231.

```
pars <- .set_pars("Bailey2001")</pre>
```

ExampleData.ModelOutput

Example data (TL curve) simulated with parameter set from Pagonis 2007

Description

Example data (TL curve) simulated with parameter set from Pagonis 2007

Format

A RLum. Analysis object containing one TL curve as RLum. Data. Curve.

Function version

0.1.1

Note

```
This example has only one record (TL). The used sequence was sequence <- list(IRR = c(temp = 20, dose = 10, DoseRate = 1), TL = c(temp_begin = 20, temp_end = 400, heating_rate = 5))
```

Author(s)

Johannes Friedrich, University of Bayreuth (Germany)

Source

```
model_LuminescenceSignals()
```

References

Pagonis, V., Chen, R., Wintle, A.G., 2007: Modelling thermal transfer in optically stimulated luminescence of quartz. Journal of Physics D: Applied Physics 40, 998-1006.

```
data("ExampleData.ModelOutput", envir = environment())

TL_curve <- get_RLum(model.output, recordType = "TL$", drop = FALSE)

##plot TL curve
plot_RLum(TL_curve)

TL_concentrations <- get_RLum(model.output, recordType = "(TL)", drop = FALSE)
plot_RLum(TL_concentrations)</pre>
```

```
model_LuminescenceSignals
```

Model Luminescence Signals

Description

This function models luminescence signals for quartz based on published physical models. It is possible to simulate TL, (CW-) OSL, RF measurements in a arbitrary sequence. This sequence is defined as a list of certain aberrations. Furthermore it is possible to load a sequence direct from the Risø Sequence Editor. The output is an Luminescence::RLum.Analysis object and so the plots are done by the Luminescence::plot_RLum.Analysis function. If a SAR sequence is simulated the plot output can be disabled and SAR analyse functions can be used.

Usage

```
model_LuminescenceSignals(
  model,
  sequence,
  lab.dose_rate = 1,
  simulate_sample_history = FALSE,
  plot = TRUE,
  verbose = TRUE,
  show_structure = FALSE,
  own_parameters = NULL,
  own_state_parameters = NULL,
  own_start_temperature = NULL,
  ...
)
```

Arguments

model character (**required**): set model to be used. Available models are: "Bailey2001",

"Bailey2002", "Bailey2004", "Pagonis2007", "Pagonis2008", "Friedrich2017", "Friedrich2018", "Peng2022" and for own models "customized" (or "customised"). Note: When model = "customized"/"customised is set, the argument own_parameters

has to be set.

sequence list (required): set sequence to model as list or as *.seq file from the Risø

sequence editor. To simulate SAR measurements there is an extra option to set

the sequence list (cf. details).

lab.dose_rate numeric (with default): laboratory dose rate in XXX Gy/s for calculating sec-

onds into Gray in the *.seq file.

simulate_sample_history

logical (with default): FALSE (with default): simulation begins at laboratory conditions, TRUE: simulations begins at crystallization process (all levels 0)

plot logical (with default): Enables or disables plot output

verbose logical (with default): Verbose mode on/off

show_structure logical (with default): Shows the structure of the result. Recommended to show

record. id to analyse concentrations.

own_parameters list (with default): This argument allows the user to submit own parameter sets. See details for more information.

own_state_parameters

numeric (with default): Some publications (e.g., Pagonis 2009) offer state parameters. With this argument the user can submit this state parameters. For further details see vignette "RLumModel - Using own parameter sets" and example 3. The parameter also accepts an Luminescence::RLum.Results object created by .set_pars as input.

own_start_temperature

numeric (with default): Parameter to control the start temperature (in °C) of a simulation. This parameter takes effect only when 'model = "customized"' is chosen.

further arguments and graphical parameters passed to plot.default. See details for further information.

Details

Defining a sequence

Arguments	Description	Sub-arguments
TL	thermally stimulated luminescence	'temp begin' (°C), 'temp end' (°C), 'heating rate' (°C/s)
OSL	optically stimulated luminescence	'temp' (°C), 'duration' (s), 'optical_power' (%)
ILL	illumination	'temp' (°C), 'duration' (s), 'optical_power' (%)
LM_OSL	linear modulated OSL	'temp' (°C), 'duration' (s), optional: 'start_power' (%), 'end_power'
RL/RF	radioluminescence	'temp' (°C), 'dose' (Gy), 'dose_rate' (Gy/s)
RF_heating	RF during heating/cooling	'temp begin' (°C), 'temp end' (°C), 'heating rate' (°C/s], 'dose_rate'
IRR	irradiation	'temp' (°C), 'dose' (Gy), 'dose_rate' (Gy/s)
CH	cutheat	'temp' (°C), optional: 'duration' (s), 'heating_rate' (°C/s)
PH	preheat	'temp' (°C), 'duration' (s), optional: 'heating_rate' (°C/s)
PAUSE	pause	'temp' (°C), 'duration' (s)

Note: 100% illumination power equates to 20 mW/cm^2

Own parameters

The list has to contain the following items:

- N: Concentration of electron- and hole traps (cm^(-3))
- E: Electron/Hole trap depth (eV)
- s: Frequency factor (s^(-1))
- A: Conduction band to electron trap and valence band to hole trap transition probability (s^(-1) * cm^(3)). CAUTION: Not every publication uses the same definition of parameter A and B! See vignette "RLumModel Usage with own parameter sets" for further details
- B: Conduction band to hole centre transition probability (s^(-1) * cm^(3)).
- Th: Photo-eviction constant or photoionisation cross section, respectively
- E_th: Thermal assistence energy (eV)
- k_B: Boltzman constant 8.617e-05 (eV/K)
- W: activation energy 0.64 (eV) (for UV)
- K: 2.8e7 (dimensionless constant)
- model: "customized"

• R (optional): Ionisation rate (pair production rate) equivalent to 1 Gy/s (s^(-1)) * cm^(-3))

For further details see Bailey 2001, Wintle 1975, vignette "RLumModel - Using own parameter sets" and example 3.

Defining a SAR-sequence

Abrivation	Description	examples
RegDose	Dose points of the regenerative cycles (Gy)	c(0, 80, 140, 260, 320, 0, 80)
TestDose	Test dose for the SAR cycles (Gy)	50
PH	Temperature of the preheat (°C)	240
CH	Temperature of the cutheat (°C)	200
OSL_temp	Temperature of OSL read out (°C)	125
OSL_duration	Duration of OSL read out (s)	default: 40
Irr_temp	Temperature of irradiation (°C)	default: 20
PH_duration	Duration of the preheat (s)	default: 10
dose_rate	Dose rate of the laboratory irradiation source (Gy/s)	default: 1
optical_power	Percentage of the full illumination power (%)	default: 90
Irr_2recover	Dose to be recovered in a dose-recovery-test (Gy)	20

Value

This function returns an Luminescence::RLum.Analysis object with all TL, (LM-) OSL and RF/RL steps in the sequence. Every entry is an Luminescence::RLum.Data.Curve object and can be plotted, analysed etc. with further RLum-functions.

Function version

0.1.6

How to cite

Friedrich, J., Kreutzer, S., 2022. model_LuminescenceSignals(): Model Luminescence Signals. Function version 0.1.6. In: Friedrich, J., Kreutzer, S., Schmidt, C., 2022. RLumModel: Solving Ordinary Differential Equations to Understand Luminescence. R package version 0.2.10. https://CRAN.R-project.org/package=RLumModel

Author(s)

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References

Bailey, R.M., 2001. Towards a general kinetic model for optically and thermally stimulated luminescence of quartz. Radiation Measurements 33, 17-45.

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Bailey, R.M., 2004. Paper I-simulation of dose absorption in quartz over geological timescales and it simplications for the precision and accuracy of optical dating. Radiation Measurements 38, 299-310.

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Pagonis, V., Chen, R., Wintle, A.G., 2007: Modelling thermal transfer in optically stimulated luminescence of quartz. Journal of Physics D: Applied Physics 40, 998-1006.

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Peng, J., Wang, X., Adamiec, G., 2022. The build-up of the laboratory-generated dose-response curve and underestimation of equivalent dose for quartz OSL in the high dose region: A critical modelling study. Quaternary Geochronology 67, 101231.

Soetaert, K., Cash, J., Mazzia, F., 2012. Solving differential equations in R. Springer Science & Business Media.

Wintle, A., 1975. Thermal Quenching of Thermoluminescence in Quartz. Geophysical Journal International 41, 107-113.

See Also

```
plot, Luminescence::RLum, read_SEQ2R
```

```
## Example 1: Simulate Bailey2001
## (cf. Bailey, 2001, Fig. 1)
##set sequence with the following steps
## (1) Irradiation at 20 deg. C with a dose of 10 Gy and a dose rate of 1 Gy/s
## (2) TL from 20-400 deg. C with a rate of 5 K/s
sequence <-
  list(
   IRR = c(20, 10, 1),
   TL = c(20, 400, 5)
  )
##model sequence
model.output <- model_LuminescenceSignals(</pre>
  sequence = sequence,
  model = "Bailey2001"
##get all TL concentrations
TL_conc <- get_RLum(model.output, recordType = "(TL)", drop = FALSE)</pre>
plot_RLum(TL_conc)
```

```
##plot 110 deg. C trap concentration
TL_110 <- get_RLum(TL_conc, recordType = "conc. level 1")
plot_RLum(TL_110)
##===========================##
## Example 2: compare different optical powers of stimulation light
# call function "model_LuminescenceSignals", model = "Bailey2004"
# and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence
# the optical_power of the LED is varied and then compared.
optical_power <- seq(from = 0, to = 100, by = 20)</pre>
model.output <- lapply(optical_power, function(x){</pre>
 sequence <- list(IRR = c(20, 50, 1),
                PH = c(220, 10, 5),
                OSL = c(125, 50, x)
                )
 data <- model_LuminescenceSignals(</pre>
         sequence = sequence,
          model = "Bailey2004",
          plot = FALSE,
          verbose = FALSE
return(get_RLum(data, recordType = "OSL$", drop = FALSE))
})
##combine output curves
model.output.merged <- merge_RLum(model.output)</pre>
##plot
plot_RLum(
object = model.output.merged,
xlab = "Illumination time (s)",
ylab = "OSL signal (a.u.)",
main = "OSL signal dependency on optical power of stimulation light",
 legend.text = paste("Optical power density", 20*optical_power/100, "mW/cm^2"),
combine = TRUE)
## Example 3: Usage of own parameter sets (Pagonis 2009)
##_____##
own_parameters <- list(</pre>
 N = c(2e15, 2e15, 1e17, 2.4e16),
 E = c(0, 0, 0, 0),
 s = c(0, 0, 0, 0),
 A = c(2e-8, 2e-9, 4e-9, 1e-8),
 B = c(0, 0, 5e-11, 4e-8),
 Th = c(0, 0),
 E_{th} = c(0, 0),
```

```
k_B = 8.617e-5,
 W = 0.64,
 K = 2.8e7
 model = "customized",
 R = 1.7e15
## Note: In Pagonis 2009 is B the valence band to hole centre probability,
## but in Bailey 2001 this is A_j. So the values of B (in Pagonis 2009)
## are A in the notation above. Also notice that the first two entries in N, A and
## B belong to the electron traps and the last two entries to the hole centres.
own_state_parameters <- c(0, 0, 0, 9.4e15)
## calculate Fig. 3 in Pagonis 2009. Note: The labels for the dose rate in the original
## publication are not correct.
## For a dose rate of 0.1 Gy/s belongs a RF signal to ~ 1.5e14 (see Fig. 6).
sequence <- list(RF = c(20, 0.1, 0.1))
model_LuminescenceSignals(
  model = "customized",
  sequence = sequence,
  own_parameters = own_parameters,
  own_state_parameters = own_state_parameters)
## Not run:
## Example 4: Simulate Thermal-Activation-Characteristics (TAC)
##set temperature
act.temp <- seq(from = 80, to = 600, by = 20)
##loop over temperature
model.output <- vapply(X = act.temp, FUN = function(x) {</pre>
##set sequence, note: sequence includes sample history
  sequence <- list(</pre>
    IRR = c(20, 1, 1e-11),
    IRR = c(20, 10, 1),
    PH = c(x, 1),
    IRR = c(20, 0.1, 1),
    TL = c(20, 150, 5)
##run simulation
  temp <- model_LuminescenceSignals(</pre>
    sequence = sequence,
    model = "Pagonis2007",
    simulate_sample_history = TRUE,
    plot = FALSE,
    verbose = FALSE
  )
    ## "TL$" for exact matching TL and not (TL)
  TL_curve <- get_RLum(temp, recordType = "TL$")</pre>
```

```
##return max value in TL curve
   return(max(get_RLum(TL_curve)[,2]))
 }, FUN. VALUE = 1)
 ##plot resutls
 plot(
  act.temp[-(1:3)],
  model.output[-(1:3)],
  type = "b",
  xlab = "Temperature [\u00B0C)",
  ylab = "TL [a.u.]"
##===========================##
## Example 5: Simulate SAR sequence
##===========================##
##set SAR sequence with the following steps
## (1) RegDose: set regenerative dose (Gy) as vector
## (2) TestDose: set test dose (Gy)
## (3) PH: set preheat temperature in deg. C
## (4) CH: Set cutheat temperature in deg. C
## (5) OSL_temp: set OSL reading temperature in deg. C
## (6) OSL_duration: set OSL reading duration in s
sequence <- list(</pre>
RegDose = c(0,10,20,50,90,0,10),
TestDose = 5,
PH = 240,
CH = 200,
OSL_{temp} = 125,
OSL_duration = 70)
# call function "model_LuminescenceSignals", set sequence = sequence,
# model = "Pagonis2007" (palaeodose = 20 Gy) and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence
model.output <- model_LuminescenceSignals(</pre>
   sequence = sequence,
  model = "Pagonis2007",
  plot = FALSE
# in environment is a new object "model.output" with the results of
# every step of the given sequence.
\mbox{\# Plots} are done at OSL and TL steps and the growth curve
# call "analyse_SAR.CWOSL" from RLum package
 results <- analyse_SAR.CWOSL(model.output,</pre>
                           signal.integral.min = 1,
                           signal.integral.max = 15,
                           background.integral.min = 601,
                           background.integral.max = 701,
                           fit.method = "EXP",
                           dose.points = c(0,10,20,50,90,0,10))
```

```
## Example 6: generate sequence from *.seq file and run SAR simulation
# load example *.SEQ file and construct a sequence.
# call function "model_LuminescenceSignals", load created sequence for sequence,
# set model = "Bailey2002" (palaeodose = 10 Gy)
# and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence
path <- system.file("extdata", "example_SAR_cycle.SEQ", package="RLumModel")</pre>
sequence <- read_SEQ2R(file = path)</pre>
model.output <- model_LuminescenceSignals(</pre>
 sequence = sequence,
 model = "Bailey2001",
 plot = FALSE
## call RLum package function "analyse_SAR.CWOSL" to analyse the simulated SAR cycle
results <- analyse_SAR.CWOSL(model.output,
                         signal.integral.min = 1,
                         signal.integral.max = 10,
                         background.integral.min = 301,
                         background.integral.max = 401,
                         dose.points = c(0,8,14,26,32,0,8),
                         fit.method = "EXP")
print(get_RLum(results))
## Example 7: Simulate sequence at laboratory without sample history
##=========================##
##set sequence with the following steps
## (1) Irraditation at 20 deg. C with a dose of 100 Gy and a dose rate of 1 Gy/s
## (2) Preheat to 200 deg. C and hold for 10 s
## (3) LM-OSL at 125 deg. C. for 100 s
## (4) Cutheat at 200 dec. C.
## (5) Irraditation at 20 deg. C with a dose of 10 Gy and a dose rate of 1 Gy/s
## (6) Pause at 200 de. C. for 100 s
## (7) OSL at 125 deg. C for 100 s with 90 % optical power
## (8) Pause at 200 deg. C for 100 s
## (9) TL from 20-400 deg. C with a heat rate of 5 K/s
## (10) Radiofluorescence at 20 deg. C with a dose of 200 Gy and a dose rate of 0.01 Gy/s
sequence <-
list(
  IRR = c(20, 100, 1),
  PH = c(200, 10),
  LM_{OSL} = c(125, 100),
  CH = c(200),
  IRR = c(20, 10, 1),
```

14 read_SEQ2R

```
PAUSE = c(200, 100),
  OSL = c(125, 100, 90),
  PAUSE = c(200, 100),
  TL = c(20, 400, 5),
  RF = c(20, 200, 0.01)
)

# call function "model_LuminescenceSignals", set sequence = sequence,
# model = "Pagonis2008" (palaeodose = 200 Gy) and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence

model.output <- model_LuminescenceSignals(
    sequence = sequence,
    model = "Pagonis2008"
    )

## End(Not run)</pre>
```

read_SEQ2R

Parse a Risoe SEQ-file to a sequence neccessary for simulating quartz luminescence

Description

A SEQ-file created by the Risoe Sequence Editor can be imported to simulate the sequence written in the sequence editor.

Usage

```
read_SEQ2R(file, lab.dose_rate = 1, txtProgressBar = TRUE)
```

Arguments

file character (**required**): a *.seq file created by the Risoe Sequence Editor

lab.dose_rate character (with default): set the dose rate of the radiation source in the laboratory Gy/s. Default: 1 Gy/s

txtProgressBar logical (with default): enables or disables the txtProgressBar for a visuell control of the progress. Default: txtProgressBar = TRUE

Details

Supported versions: Supppored and tested: version 4.36.

Value

This function returns a list with the parsed *.seq file and the required steps for model_LuminescenceSignals.

Function version

0.1.0

How to cite

Friedrich, J., 2022. read_SEQ2R(): Parse a Risoe SEQ-file to a sequence neccessary for simulating quartz luminescence. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Schmidt, C., 2022. RLumModel: Solving Ordinary Differential Equations to Understand Luminescence. R package version 0.2.10. https://CRAN.R-project.org/package=RLumModel

Author(s)

Johannes Friedrich, University of Bayreuth (Germany),

References

Riso: Sequence Editor User Manual. Available at: http://www.nutech.dtu.dk/english/-/media/Andre_Universitetsenheder SequenceEditor.ashx?la=da

See Also

```
model_LuminescenceSignals, readLines
```

Examples

```
##search "example_SAR_cycle.SEQ" in "extdata" in package "RLumModel"
path <- system.file("extdata", "example_SAR_cycle.SEQ", package="RLumModel")
sequence <- read_SEQ2R(file = path, txtProgressBar = FALSE)</pre>
```

trace_ParameterStateEvolution

Trace parameter state evolution

Description

Traces the evolution of the concentrations in the different levels over different simulation steps. For instance, a sequence consisting of one TL and one OSL step has two iterations. For each step the end concentration is extracted. This way, the evolution of the system can be traced throughout a sequence.

Usage

```
trace_ParameterStateEvolution(object, step = NULL, plot = TRUE, ...)
```

Arguments

object	Luminescence::RLum.Analysis (required): input object created by the function model_LuminescenceSignals. The input can be a list of such objects	
step	character (optional): filter the input object to pick particular steps, the input is passed to Luminescence::get_RLum	
plot	logical (with default): enables/disables plot output	
	optional arguments to be passed to control the plot output. Supported are xlim, xlab, ylab, log, col, type, bg, main, norm (TRUE/FALSE), grid (TRUE/FALSE), step_names (TRUE/FALSE) Where meaningful, parameters can be provided as vectors. Vectors short than the number of plots are recycled.	

Value

Returns a plot and list with matrix objects of the parameter evolution. If object is a list the output is a nested list

Function version

0.1.0

How to cite

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```
sequence <-
list(
IRR = c(20, 10, 1),
TL = c(20, 400, 5),
IRR = c(20, 10, 1),
TL = c(20, 400, 5))

##model sequence
model.output <- model_LuminescenceSignals(
    sequence = sequence,
    verbose = FALSE,
    plot = FALSE,
    model = "Bailey2001")

## trace
trace_ParameterStateEvolution(model.output)</pre>
```

Index

```
* datasets
    ExampleData.ModelOutput, 5
* package
    RLumModel-package, 2
.set_pars, 3, 7
character, 3, 6, 14, 15
ExampleData.ModelOutput, 5
list, 3, 6, 7, 14, 16
logical, 6, 14, 15
Luminescence::get_RLum, 15
Luminescence::plot_RLum.Analysis, 6
Luminescence::RLum,9
Luminescence::RLum.Analysis, 6, 8, 15
Luminescence::RLum.Data.Curve, 8
Luminescence::RLum.Results,7
matrix, 16
model.output (ExampleData.ModelOutput),
model_LuminescenceSignals, 4, 6, 14, 15
numeric, 6, 7
plot, 9
plot.default, 7
read_SEQ2R, 9, 14
readLines, 15
RLumModel-package, 2
trace_ParameterStateEvolution, 15
```