

Package ‘RLumModel’

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Type Package

Title Solving Ordinary Differential Equations to Understand Luminescence

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Description A collection of functions to simulate luminescence signals in quartz and Al₂O₃ based on published models.

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BugReports <https://github.com/R-Lum/RLumModel/issues>

Depends R (>= 3.6.0),
utils,
Luminescence (>= 0.9.0)

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khroma (>= 1.7.0),
methods,
Rcpp (>= 1.0.6)

Suggests testthat (>= 3.0.0),
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URL <https://CRAN.R-project.org/package=RLumModel>

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| RLumModel-package | <i>Solving Ordinary Differential Equations to Understand Luminescence</i> |
|-------------------|---|

Description

Details

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

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Project source code repository

- <https://github.com/R-Lum/RLumModel>

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

`model` **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

How to cite

Friedrich, J., 2022. .set_pars(): Set parameters for Different Quartz Luminescence Models. Function version 0.1.3. In: Friedrich, J., Kreutzer, S., Schmidt, C., 2022. RLumModel: Solving Ordinary Differential Equations to Understand Luminescence. R package version 0.2.10.9000-35. <https://CRAN.R-project.org/package=RLumModel>

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.
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- 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.

Examples

```
pars <- .set_pars("Bailey2001")
```

`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.

Examples

```
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)
```

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 (<i>with default</i>): laboratory dose rate in XXX Gy/s for calculating seconds 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.

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' (Gy/s) |
| 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/cm²

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 * cm³). **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 * cm³).
- Th: Photo-eviction constant or photoionisation cross section, respectively
- E_th: Thermal assistance 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

0.1.5

How to cite

Friedrich, J., Kreutzer, S., 2022. model_LuminescenceSignals(): Model Luminescence Signals. Function version 0.1.5. In: Friedrich, J., Kreutzer, S., Schmidt, C., 2022. RLumModel: Solving Ordinary Differential Equations to Understand Luminescence. R package version 0.2.10.9000-35. <https://CRAN.R-project.org/package=RLumModel>

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, Geography & Earth Sciences, Aberystwyth University (United Kingdom)

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

See Also

[plot, Luminescence::RLum, read_SEQ2R](#)

Examples

```
##=====##
## 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(
  sequence = sequence,
  model = "Bailey2001"
)

##get all TL concentrations

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

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)

model.output <- lapply(optical_power, function(x){

  sequence <- list(IRR = c(20, 50, 1),
                    PH = c(220, 10, 5),
                    OSL = c(125, 50, x)
                  )

  data <- model_LuminescenceSignals(
    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)

##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(
  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) {

  ##set sequence, note: sequence includes sample history
  sequence <- list(
    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(
    sequence = sequence,
    model = "Pagonis2007",
    simulate_sample_history = TRUE,
    plot = FALSE,
    verbose = FALSE
  )

  ## "TL$" for exact matching TL and not (TL)
  TL_curve <- get_RLum(temp, recordType = "TL$")
  ##return max value in TL curve
  return(max(get_RLum(TL_curve)[,2]))
}, FUN.VALUE = 1)

```

```

##plot results
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(
  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(
  sequence = sequence,
  model = "Pagonis2007",
  plot = FALSE
)

# in environment is a new object "model.output" with the results of
# every step of the given sequence.
# 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,
  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")

sequence <- read_SEQ2R(file = path)

model.output <- model_LuminescenceSignals(
  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) Irradiation 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) Irradiation 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),
  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)

```

| | |
|------------|--|
| read_SEQ2R | <i>Parse a Risoe SEQ-file to a sequence necessary for simulating quartz luminescence</i> |
|------------|--|

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 visuall 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 necessary 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 0.2.10.9000-35. <https://CRAN.R-project.org/package=RLumModel>

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References

Riso: Sequence Editor User Manual. Available at: http://www.nutech.dtu.dk/english/-/media/Andre_Universitetsenheden/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)
```

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 (<i>optional</i>): filter the input object to pick particular steps, the input is passed to Luminescence::get_RLum |
| plot | logical (<i>with default</i>): enables/disables plot output |
| ... | optional arguments to be passed to control the plot output. Supported are xlab, ylab, col, type, bg, main, grid (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

Kreutzer, S., 2022. `trace_ParameterStateEvolution()`: Trace parameter state evolution. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Schmidt, C., 2022. *RLumModel: Solving Ordinary Differential Equations to Understand Luminescence*. R package version 0.2.10.9000-35. <https://CRAN.R-project.org/package=RLumModel>

Author(s)

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Examples

```
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)
```


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