

Package ‘babelmixr2’

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Type Package

Title Use 'nlmixr2' to Interact with Open Source and Commercial Software

Version 0.1.7

Description Run other estimation and simulation software via the 'nlmixr2' (Fidler et al (2019) <[doi:10.1002/psp4.12445](https://doi.org/10.1002/psp4.12445)>) interface including 'PKNCA', 'NONMEM' and 'Monolix'. While not required, you can get/install the 'lixoftConnectors' package in the 'Monolix' installation, as described at the following url <<https://monolixsuite.slp-software.com/r-functions/2024R1/installation-and-initialization>>. When 'lixoftConnectors' is available, 'Monolix' can be run directly instead of setting up command line usage.

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URL <https://nlmixr2.github.io/babelmixr2/>,
<https://github.com/nlmixr2/babelmixr2/>

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Contents

.setupPopEDdatabase	2
as.nlmixr2	3
babel.poped.database	5
babelBpopIdx	5
bbIDatToMonolix	7
getStandardColNames	10
modelUnitConversion	10
monolixControl	11
nlmixr2Est.pknca	14
nonmemControl	15
pkncaControl	18
popedControl	19
popedGetMultipleEndpointModelingTimes	30
popedMultipleEndpointResetTimeIndex	31
rxToMonolix	32
rxToNonmem	32
simplifyUnit	33

Index 34

.setupPopEDdatabase *Setup the poped database*

Description

Setup the poped database

Usage

```
.setupPopEDdatabase(ui, data, control)
```

Arguments

ui	rxode2 ui function
data	babelmixr2 design data
control	PopED control

Value

PopED database

Author(s)

Matthew L. Fidler

as.nlmixr2

Convert an object to a nlmixr2 fit object

Description

Convert an object to a nlmixr2 fit object

Usage

```
as.nlmixr2(  
  x,  
  ...,  
  table = nlmixr2est::tableControl(),  
  rxControl = rxode2::rxControl(),  
  ci = 0.95  
)
```

```
as.nlmixr(  
  x,  
  ...,  
  table = nlmixr2est::tableControl(),  
  rxControl = rxode2::rxControl(),  
  ci = 0.95  
)
```

Arguments

x	Object to convert
...	Other arguments
table	is the nlmixr2est::tableControl() options
rxControl	is the rxode2::rxControl() options, which is generally needed for how addl doses are handled in the translation
ci	is the confidence interval of the residual differences calculated (by default 0.95)

Value

nlmixr2 fit object

Author(s)

Matthew L. Fidler

Examples

```

# First read in the model (but without residuals)
mod <- nonmem2rx(system.file("mods/cpt/runODE032.ct1", package="nonmem2rx"),
                 determineError=FALSE, lst=".res", save=FALSE)

# define the model with residuals (and change the name of the
# parameters) In this step you need to be careful to not change the
# estimates and make sure the residual estimates are correct (could
# have to change var to sd).

mod2 <-function() {
  ini({
    lcl <- 1.37034036528946
    lvc <- 4.19814911033061
    lq <- 1.38003493562413
    lvp <- 3.87657341967489
    RSV <- c(0, 0.196446108190896, 1)
    eta.cl ~ 0.101251418415006
    eta.v ~ 0.0993872449483344
    eta.q ~ 0.101302674763154
    eta.v2 ~ 0.0730497519364148
  })
  model({
    cmt(CENTRAL)
    cmt(PERI)
    cl <- exp(lcl + eta.cl)
    v <- exp(lvc + eta.v)
    q <- exp(lq + eta.q)
    v2 <- exp(lvp + eta.v2)
    v1 <- v
    scale1 <- v
    k21 <- q/v2
    k12 <- q/v
    d/dt(CENTRAL) <- k21 * PERI - k12 * CENTRAL - cl * CENTRAL/v1
    d/dt(PERI) <- -k21 * PERI + k12 * CENTRAL
    f <- CENTRAL/scale1
    f ~ prop(RSV)
  })
}

# now we create another nonmem2rx object that validates the model above:

new <- as.nonmem2rx(mod2, mod)

# once that is done, you can translate to a full.nlmixr2 fit (if you wish)

```

```
fit <- as.nlmixr2(new)
print(fit)
```

babel.poped.database *Expand a babelmixr2 PopED database*

Description

Expand a babelmixr2 PopED database

Usage

```
babel.poped.database(popedInput, ..., optTime = NA)
```

Arguments

popedInput	The babelmixr2 generated PopED database
...	other parameters sent to PopED::create.poped.database()
optTime	boolean to indicate if the global time indexer inside of babelmixr2 is reset if the times are different. By default this is TRUE. If FALSE you can get slightly better run times and possibly slightly different results. When optTime is FALSE the global indexer is reset every time the PopED rxode2 is setup for a problem or when a poped dataset is created. You can manually reset with popedMultipleEndpointResetTimeIndex

Value

babelmixr2 PopED database (with \$babelmixr2 in database)

Author(s)

Matthew L. Fidler

babelBpopIdx	<i>Get the bpop_idx by variable name for a poped database created by babelmixr2</i>
--------------	---

Description

This may work for other poped databases if the population parameters are named.

Usage

```
babelBpopIdx(popedInput, var)
```

Arguments

popedInput The babelmixr2 created database
var variable to query

Value

index of the variable

Author(s)

Matthew L. Fidler

Examples

```
if (requireNamespace("PopED", quietly=TRUE)) {

f <- function() {
  ini({
    tV <- 72.8
    tKa <- 0.25
    tCl <- 3.75
    tF <- fix(0.9)
    pedCL <- 0.8

    eta.v ~ 0.09
    eta.ka ~ 0.09
    eta.cl ~0.25^2

    prop.sd <- fix(sqrt(0.04))
    add.sd <- fix(sqrt(5e-6))

  })
  model({
    V<-tV*exp(eta.v)
    KA<-tKa*exp(eta.ka) * (pedCL**isPediatric) # add covariate for pediatrics
    CL<-tCl*exp(eta.cl)
    Favail <- tF

    N <- floor(t/TAU)+1
    y <- (DOSE*Favail/V)*(KA/(KA - CL/V)) *
      (exp(-CL/V * (t - (N - 1) * TAU)) *
        (1 - exp(-N * CL/V * TAU))/(1 - exp(-CL/V * TAU)) -
        exp(-KA * (t - (N - 1) * TAU)) * (1 - exp(-N * KA * TAU))/(1 - exp(-KA * TAU)))

    y ~ prop(prop.sd) + add(add.sd)
  })
}

e <- et(c( 1,8,10,240,245))

babel.db <- nlmixr2(f, e, "poped",
```

```

        popedControl(m = 2,
                    groupsize=20,
                    bUseGrouped_xt=TRUE,
                    a=list(c(DOSE=20,TAU=24,isPediatric = 0),
                          c(DOSE=40, TAU=24,isPediatric = 0)))

    babelBpopIdx(babel.db, "pedCL")

}

```

bblDatToMonolix	<i>Convert nlmixr2-compatible data to other formats (if possible)</i>
-----------------	---

Description

Convert nlmixr2-compatible data to other formats (if possible)

Usage

```

bblDatToMonolix(
  model,
  data,
  table = nlmixr2est::tableControl(),
  rxControl = rxode2::rxControl(),
  env = NULL
)

```

```

bblDatToNonmem(
  model,
  data,
  table = nlmixr2est::tableControl(),
  rxControl = rxode2::rxControl(),
  env = NULL
)

```

```

bblDatToRxode(
  model,
  data,
  table = nlmixr2est::tableControl(),
  rxControl = rxode2::rxControl(),
  env = NULL
)

```

```

bblDatToMrgsolve(
  model,
  data,
  table = nlmixr2est::tableControl(),
  rxControl = rxode2::rxControl(),
)

```

```

    env = NULL
  )

  bbIDatToPknca(
    model,
    data,
    table = nlmixr2est::tableControl(),
    rxControl = rxode2::rxControl(),
    env = NULL
  )

```

Arguments

model	rxode2 model for conversion
data	Input dataset.
table	is the table control; this is mostly to figure out if there are additional columns to keep.
rxControl	is the rxode2 control options; This is to figure out how to handle the addl dosing information.
env	When NULL (default) nothing is done. When an environment, the function <code>nlmixr2est::.foceiPreProc</code> env, model, rxControl) is called on the provided environment.

Value

With the function `bbIDatToMonolix()` return a list with:

- Monolix compatible dataset (`$monolix`)
- Monolix ADM information (`$adm`)

With the function `nlmixrDataToNonmem()` return a dataset that is compatible with NONMEM.

With the function `nlmixrDataToMrgsolve()` return a dataset that is compatible with mrgsolve. Unlike NONMEM, it supports replacement events with `evid=8` (note with rxode2 replacement `evid` is 5).

With the function `nlmixrDataToRxode()` this will normalize the dataset to use newer `evid` definitions that are closer to NONMEM instead of any classic definitions that are used at a lower level

Author(s)

Matthew L. Fidler

Examples

```

pk.turnover.emax3 <- function() {
  ini({
    tktr <- log(1)
    tka <- log(1)
    tcl <- log(0.1)
    tv <- log(10)
  })
}

```



```

##
eta.ktr ~ 1
eta.ka ~ 1
eta.cl ~ 2
eta.v ~ 1
prop.err <- 0.1
pkadd.err <- 0.1
##
temax <- logit(0.8)
tec50 <- log(0.5)
tkout <- log(0.05)
te0 <- log(100)
##
eta.emax ~ .5
eta.ec50 ~ .5
eta.kout ~ .5
eta.e0 ~ .5
##
pdadd.err <- 10
})
model({
  ktr <- exp(tktr + eta.ktr)
  ka <- exp(tka + eta.ka)
  cl <- exp(tcl + eta.cl)
  v <- exp(tv + eta.v)
  emax = expit(temax+eta.emax)
  ec50 = exp(tec50 + eta.ec50)
  kout = exp(tkout + eta.kout)
  e0 = exp(te0 + eta.e0)
  ##
  DCP = center/v
  PD=1-emax*DCP/(ec50+DCP)
  ##
  effect(0) = e0
  kin = e0*kout
  ##
  d/dt(depot) = -ktr * depot
  d/dt(gut) = ktr * depot -ka * gut
  d/dt(center) = ka * gut - cl / v * center
  d/dt(effect) = kin*PD -kout*effect
  ##
  cp = center / v
  cp ~ prop(prop.err) + add(pkadd.err)
  effect ~ add(pdadd.err) | pca
})
}

bblDatToMonolix(pk.turnover.emax3, nlmixr2data::warfarin)

bblDatToNonmem(pk.turnover.emax3, nlmixr2data::warfarin)

bblDatToMrgsolve(pk.turnover.emax3, nlmixr2data::warfarin)

```

```
bb1DatToRxode(pk.turnover.emax3, nlmixr2data::warfarin)
```

```
getStandardColNames     Determine standardized rxode2 column names from data
```

Description

Determine standardized rxode2 column names from data

Usage

```
getStandardColNames(data)
```

Arguments

data A data.frame as the source for column names

Value

A named character vector where the names are the standardized names and the values are either the name of the column from the data or NA if the column is not present in the data.

Examples

```
getStandardColNames(data.frame(ID=1, DV=2, Time=3, CmT=4))
```

```
modelUnitConversion     Unit conversion for pharmacokinetic models
```

Description

Unit conversion for pharmacokinetic models

Usage

```
modelUnitConversion(
  dvu = NA_character_,
  amtu = NA_character_,
  timeu = NA_character_,
  volumeu = NA_character_
)
```

Arguments

dvu, amtu, timeu The units for the DV, AMT, and TIME columns in the data
 volumeu The units for the volume parameters in the model

Value

A list with names for the units associated with each parameter ("amtu", "clearanceu", "volumeu", "timeu", "dvu") and the numeric value to multiply the modeled estimate (for example, cp) so that the model is consistent with the data units.

See Also

Other Unit conversion: [simplifyUnit\(\)](#)

Examples

```
modelUnitConversion(dvu = "ng/mL", amtu = "mg", timeu = "hr", volumeu = "L")
```

monolixControl

Monolix Controller for nlmixr2

Description

Monolix Controller for nlmixr2

Usage

```
monolixControl(  
  nbSSDoses = 7,  
  useLinearization = FALSE,  
  stiff = FALSE,  
  addProp = c("combined2", "combined1"),  
  exploratoryAutoStop = FALSE,  
  smoothingAutoStop = FALSE,  
  burnInIterations = 5,  
  smoothingIterations = 200,  
  exploratoryIterations = 250,  
  simulatedAnnealingIterations = 250,  
  exploratoryInterval = 200,  
  exploratoryAlpha = 0,  
  omegaTau = 0.95,  
  errorModelTau = 0.95,  
  variability = c("none", "firstStage", "decreasing"),  
  runCommand = getOption("babelmixr2.monolix", ""),  
  rxControl = NULL,  
  sumProd = FALSE,  
  optExpression = TRUE,  
  calcTables = TRUE,  
  compress = TRUE,  
  ci = 0.95,  
  sigdigTable = NULL,  
  absolutePath = FALSE,
```

```

modelName = NULL,
muRefCovAlg = TRUE,
run = TRUE,
...
)

```

Arguments

nbSSDoses Number of steady state doses (default 7)

useLinearization Use linearization for log likelihood and fim.

stiff boolean for using the stiff ODE solver

addProp specifies the type of additive plus proportional errors, the one where standard deviations add (combined1) or the type where the variances add (combined2).
The combined1 error type can be described by the following equation:

$$y = f + (a + b \times f^c) \times \varepsilon$$

The combined2 error model can be described by the following equation:

$$y = f + \sqrt{a^2 + b^2 \times f^{2 \times c}} \times \varepsilon$$

Where:

- y represents the observed value
- f represents the predicted value
- a is the additive standard deviation
- b is the proportional/power standard deviation
- c is the power exponent (in the proportional case c=1)

exploratoryAutoStop logical to turn on or off exploratory phase auto-stop of SAEM (default 250)

smoothingAutoStop Boolean indicating if the smoothing should automatically stop (default FALSE)

burnInIterations Number of burn in iterations

smoothingIterations Number of smoothing iterations

exploratoryIterations Number of iterations for exploratory phase (default 250)

simulatedAnnealingIterations Number of simulating annealing iterations

exploratoryInterval Minimum number of iterations in the exploratory phase (default 200)

exploratoryAlpha Convergence memory in the exploratory phase (only used when exploratoryAutoStop is TRUE)

omegaTau Proportional rate on variance for simulated annealing

errorModelTau	Proportional rate on error model for simulated annealing
variability	This describes the methodology for parameters without variability. It could be: - Fixed throughout (none) - Variability in the first stage (firstStage) - Decreasing until it reaches the fixed value (decreasing)
runCommand	is a shell command or function to run monolix; You can specify the default by <code>options("babelmixr2.monolix"="runMonolix")</code> . If it is empty and 'lixoftConnectors' is available, use <code>lixoftConnectors</code> to run monolix. See details for function usage.
rxControl	'rxode2' ODE solving options during fitting, created with <code>rxControl()</code>
sumProd	Is a boolean indicating if the model should change multiplication to high precision multiplication and sums to high precision sums using the <code>PreciseSums</code> package. By default this is FALSE.
optExpression	Optimize the rxode2 expression to speed up calculation. By default this is turned on.
calcTables	This boolean is to determine if the <code>foceiFit</code> will calculate tables. By default this is TRUE
compress	Should the object have compressed items
ci	Confidence level for some tables. By default this is 0.95 or 95% confidence.
sigdigTable	Significant digits in the final output table. If not specified, then it matches the significant digits in the 'sigdig' optimization algorithm. If 'sigdig' is NULL, use 3.
absolutePath	Boolean indicating if the absolute path should be used for the monolix runs
modelName	Model name used to generate the NONMEM output. If NULL try to infer from the model name (could be x if not clear). Otherwise use this character for outputs.
muRefCovAlg	This controls if algebraic expressions that can be mu-referenced are treated as mu-referenced covariates by: <ol style="list-style-type: none"> 1. Creating a internal data-variable 'nlmixrMuDerCov#' for each algebraic mu-referenced expression 2. Change the algebraic expression to 'nlmixrMuDerCov# * mu_cov_theta' 3. Use the internal mu-referenced covariate for saem 4. After optimization is completed, replace 'model()' with old 'model()' expression 5. Remove 'nlmixrMuDerCov#' from nlmix2 output <p>In general, these covariates should be more accurate since it changes the system to a linear compartment model. Therefore, by default this is 'TRUE'.</p>
run	Should monolix be run and the results be imported to nlmixr2? (Default is TRUE)
...	Ignored parameters

Details

If `runCommand` is given as a string, it will be called with the `system()` command like:

```
runCommand mlxtran.
```

For example, if `runCommand="/path/to/monolix/mlxbsub2021' -p "` then the command line used would look like the following:

```
'/path/to/monolix/mlxbsub2021' monolix.mlxtran
```

If `runCommand` is given as a function, it will be called as `FUN(mlxtran, directory, ui)` to run Monolix. This allows you to run Monolix in any way that you may need, as long as you can write it in R. `babelmixr2` will wait for the function to return before proceeding.

If `runCommand` is NA, `nlmixr()` will stop after writing the model files and without starting Monolix.

Note that you can get the translated monolix components from a parsed/compiled `rxode2` `ui` object with `ui$monolixModel` and `ui$mlxtran`

Value

A monolix control object

Author(s)

Matthew Fidler

nlmixr2Est.pknca	<i>Estimate starting parameters using PKNCA</i>
------------------	---

Description

Estimate starting parameters using PKNCA

Usage

```
## S3 method for class 'pknca'
nlmixr2Est(env, ...)
```

Arguments

<code>env</code>	Environment for the <code>nlmixr2</code> estimation routines. This needs to have: <ul style="list-style-type: none"> - <code>rxode2</code> <code>ui</code> object in <code>'\$ui'</code> - data to fit in the estimation routine in <code>'\$data'</code> - control for the estimation routine's control options in <code>'\$ui'</code>
<code>...</code>	Other arguments provided to <code>'nlmixr2Est()'</code> provided for flexibility but not currently used inside <code>nlmixr</code>

Details

Parameters are estimated as follows:

- ka 4 half-lives to Tmax but not higher than 3: $\log(2)/(t_{\max}/4)$
- vc Inverse of dose-normalized Cmax
- cl Estimated as the median clearance
- vp, vp22- and 4-fold the vc, respectively by default, controlled by the vpMult and vp2Mult arguments to pkncaControl
- q, q2 0.5- and 0.25-fold the cl, respectively by default, controlled by the qMult and q2Mult arguments to pkncaControl

The bounds for the parameter estimates are set to 10% of the first percentile and 10 times the 99th percentile. (For ka, the lower bound is set to the lower of 10% of the first percentile or 0.03 and the upper bound is not modified from 10 times the 99th percentile.)

Parameter estimation methods may be changed in a future version.

Value

A model with updated starting parameters. In the model a new element named "nca" will be available which includes the PKNCA results used for the calculation.

nonmemControl	<i>NONMEM estimation control</i>
---------------	----------------------------------

Description

NONMEM estimation control

Usage

```
nonmemControl(
  est = c("focei", "imp", "its", "posthoc"),
  advanOde = c("advan13", "advan8", "advan6"),
  cov = c("r,s", "r", "s", ""),
  maxeval = 1e+05,
  tol = 6,
  atol = 12,
  sstol = 6,
  ssatol = 12,
  sigl = 12,
  sigdig = 3,
  print = 1,
  extension = getOption("babelmixr2.nmModelExtension", ".nmctl"),
  outputExtension = getOption("babelmixr2.nmOutputExtension", ".lst"),
  runCommand = getOption("babelmixr2.nonmem", ""),
  iniSigDig = 5,
```

```

protectZeros = FALSE,
muRef = TRUE,
addProp = c("combined2", "combined1"),
rxControl = NULL,
sumProd = FALSE,
optExpression = TRUE,
calcTables = TRUE,
compress = TRUE,
ci = 0.95,
sigdigTable = NULL,
readRounding = FALSE,
readBadOpt = FALSE,
niter = 100L,
isample = 1000L,
iaccept = 0.4,
iscaleMin = 0.1,
iscaleMax = 10,
df = 4,
seed = 14456,
mapiter = 1,
mapinter = 0,
noabort = TRUE,
modelName = NULL,
muRefCovAlg = TRUE,
run = TRUE,
...
)

```

Arguments

<code>est</code>	NONMEM estimation method
<code>advanOde</code>	The ODE solving method for NONMEM
<code>cov</code>	The NONMEM covariance method
<code>maxeval</code>	NONMEM's maxeval (for non posthoc methods)
<code>tol</code>	NONMEM tolerance for ODE solving <code>advan</code>
<code>atol</code>	NONMEM absolute tolerance for ODE solving
<code>sstol</code>	NONMEM tolerance for steady state ODE solving
<code>ssatol</code>	NONMEM absolute tolerance for steady state ODE solving
<code>sigl</code>	NONMEM <code>sigl</code> estimation option
<code>sigdig</code>	the significant digits for NONMEM
<code>print</code>	The print number for NONMEM
<code>extension</code>	NONMEM file extensions
<code>outputExtension</code>	Extension to use for the NONMEM output listing
<code>runCommand</code>	Command to run NONMEM (typically the path to "nmfe75") or a function. See the details for more information.

iniSigDig	How many significant digits are printed in \$THETA and \$OMEGA when the estimate is zero. Also controls the zero protection numbers
protectZeros	Add methods to protect divide by zero
muRef	Automatically mu-reference the control stream
addProp, sumProd, optExpression, calcTables, compress, ci, sigdigTable	Passed to nlmixr2est::foceiControl
rxControl	Options to pass to rxode2::rxControl for simulations
readRounding	Try to read NONMEM output when NONMEM terminated due to rounding errors
readBadOpt	Try to read NONMEM output when NONMEM terminated due to an apparent failed optimization
niter	number of iterations in NONMEM estimation methods
isample	Isample argument for NONMEM ITS estimation method
iaccept	Iaccept for NONMEM ITS estimation methods
iscaleMin	parameter for IMP NONMEM method (ISCALE_MIN)
iscaleMax	parameter for IMP NONMEM method (ISCALE_MAX)
df	degrees of freedom for IMP method
seed	is the seed for NONMEM methods
mapiter	the number of map iterations for IMP method
mapinter	is the MAPINTER parameter for the IMP method
noabort	Add the NOABORT option for \$EST
modelName	Model name used to generate the NONMEM output. If NULL try to infer from the model name (could be x if not clear). Otherwise use this character for outputs.
muRefCovAlg	This controls if algebraic expressions that can be mu-referenced are treated as mu-referenced covariates by: <ol style="list-style-type: none"> 1. Creating a internal data-variable 'nlmixrMuDerCov#' for each algebraic mu-referenced expression 2. Change the algebraic expression to 'nlmixrMuDerCov# * mu_cov_theta' 3. Use the internal mu-referenced covariate for saem 4. After optimization is completed, replace 'model()' with old 'model()' expression 5. Remove 'nlmixrMuDerCov#' from nlmix2 output In general, these covariates should be more accurate since it changes the system to a linear compartment model. Therefore, by default this is 'TRUE'.
run	Should NONMEM be run (and the files imported to nlmixr2); default is TRUE, but FALSE will simply create the NONMEM control stream and data file.
...	optional genRxControl argument controlling automatic rxControl generation.

Details

If runCommand is given as a string, it will be called with the system() command like:

```
runCommand controlFile outputFile.
```

For example, if runCommand=" '/path/to/nmfe75' " then the command line used would look like the following:

```
'/path/to/nmfe75' one.cmt.nmctl one.cmt.lst
```

If runCommand is given as a function, it will be called as FUN(ctl, directory, ui) to run NONMEM. This allows you to run NONMEM in any way that you may need, as long as you can write it in R. babelmixr2 will wait for the function to return before proceeding.

If runCommand is NA, nlmixr() will stop after writing the model files and without starting NONMEM.

Value

babelmixr2 control option for generating NONMEM control stream and reading it back into babelmixr2/nlmixr2

Author(s)

Matthew L. Fidler

Examples

```
nonmemControl()
```

pkncaControl

PKNCA estimation control

Description

PKNCA estimation control

Usage

```
pkncaControl(
  concu = NA_character_,
  doseu = NA_character_,
  timeu = NA_character_,
  volumeu = NA_character_,
  vpMult = 2,
  qMult = 1/2,
  vp2Mult = 4,
  q2Mult = 1/4,
  dvParam = "cp",
  groups = character(),
  sparse = FALSE,
```

```

    ncaData = NULL,
    ncaResults = NULL,
    rxControl = rxode2::rxControl()
  )

```

Arguments

concu, doseu, timeu	concentration, dose, and time units from the source data (passed to <code>PKNCA::pknca_units_table()</code>).
volumeu	compartment volume for the model (if <code>NULL</code> , simplified units from source data will be used)
vpMult, qMult, vp2Mult, q2Mult	Multipliers for <code>vc</code> and <code>cl</code> to provide initial estimates for <code>vp</code> , <code>q</code> , <code>vp2</code> , and <code>q2</code>
dvParam	The parameter name in the model that should be modified for concentration unit conversions. It must be assigned on a line by itself, separate from the residual error model line.
groups	Grouping columns for NCA summaries by group (required if <code>sparse = TRUE</code>)
sparse	Are the concentration-time data sparse PK (commonly used in small nonclinical species or with terminal or difficult sampling) or dense PK (commonly used in clinical studies or larger nonclinical species)?
ncaData	Data to use for calculating NCA parameters. Typical use is when a subset of the original data are informative for NCA.
ncaResults	Already computed NCA results (a <code>PKNCAresults</code> object) to bypass automatic calculations. At least the following parameters must be calculated in the NCA: <code>tmax</code> , <code>cmax.dn</code> , <code>cl.last</code>
rxControl	Control options sent to <code>rxode2::rxControl()</code>

Value

A list of parameters

popedControl	<i>Control for a PopED design task</i>
--------------	--

Description

Control for a PopED design task

Usage

```

popedControl(
  stickyRecalcN = 4,
  maxOdeRecalc = 5,
  odeRecalcFactor = 10^(0.5),
  maxn = NULL,

```

```

rxControl = NULL,
sigdig = 4,
important = NULL,
unimportant = NULL,
iFIMCalculationType = c("reduced", "full", "weighted", "loc", "reducedPFIM", "fullABC",
  "largeMat", "reducedFIMABC"),
iApproximationMethod = c("fo", "foce", "focei", "foi"),
iFOCEnumInd = 1000,
prior_fim = matrix(0, 0, 1),
d_switch = c("d", "ed"),
ofv_calc_type = c("lnD", "d", "a", "Ds", "inverse"),
strEDPenaltyFile = "",
ofv_fun = NULL,
iEDCalculationType = c("mc", "laplace", "bfgs-laplace"),
ED_samp_size = 45,
bLHS = c("hypercube", "random"),
bUseRandomSearch = TRUE,
bUseStochasticGradient = TRUE,
bUseLineSearch = TRUE,
bUseExchangeAlgorithm = FALSE,
bUseBFGSMinimizer = FALSE,
bUseGrouped_xt = FALSE,
EACriteria = c("modified", "fedorov"),
strRunFile = "",
poped_version = NULL,
modtit = "PopED babelmixr2 model",
output_file = "PopED_output_summary",
output_function_file = "PopED_output_",
strIterationFileName = "PopED_current.R",
user_data = NULL,
ourzero = 1e-05,
dSeed = NULL,
line_opta = NULL,
line_optx = NULL,
bShowGraphs = FALSE,
use_logfile = FALSE,
m1_switch = c("central", "complex", "analytic", "ad"),
m2_switch = c("central", "complex", "analytic", "ad"),
hle_switch = c("central", "complex", "ad"),
gradff_switch = c("central", "complex", "analytic", "ad"),
gradfg_switch = c("central", "complex", "analytic", "ad"),
grad_all_switch = c("central", "complex"),
rsit_output = 5,
sgit_output = 1,
hm1 = 1e-05,
hlf = 1e-05,
hlg = 1e-05,
hm2 = 1e-05,

```

```
hgd = 1e-05,
hle = 1e-05,
AbsTol = 1e-06,
RelTol = 1e-06,
iDiffSolverMethod = NULL,
bUseMemorySolver = FALSE,
rsit = 300,
sgit = 150,
inrsit = 250,
intsgit = 50,
maxrsnullit = 50,
convergence_eps = 1e-08,
rslxt = 10,
rsla = 10,
cfaxt = 0.001,
cfaa = 0.001,
bGreedyGroupOpt = FALSE,
EAStepSize = 0.01,
EANumPoints = FALSE,
EAConvergenceCriteria = 1e-20,
bEANOReplicates = FALSE,
BFGSProjectedGradientTol = 1e-04,
BFGSTolerancef = 0.001,
BFGSToleranceg = 0.9,
BFGSTolerancecx = 0.1,
ED_diff_it = 30,
ED_diff_percent = 10,
line_search_it = 50,
Doptim_iter = 1,
iCompileOption = c("none", "full", "mcc", "mpi"),
compileOnly = FALSE,
iUseParallelMethod = c("mpi", "matlab"),
MCC_Dep = NULL,
strExecuteName = "calc_fim.exe",
iNumProcesses = 2,
iNumChunkDesignEvals = -2,
Mat_Out_Pre = "parallel_output",
strExtraRunOptions = "",
dPollResultTime = 0.1,
strFunctionInputName = "function_input",
bParallelRS = FALSE,
bParallelSG = FALSE,
bParallelMFEA = FALSE,
bParallelLS = FALSE,
groupsize = NULL,
time = "time",
timeLow = "low",
timeHi = "high",
```

```

id = "id",
m = NULL,
x = NULL,
ni = NULL,
maxni = NULL,
minni = NULL,
maxtotni = NULL,
mintotni = NULL,
maxgroupsize = NULL,
mingroupsize = NULL,
maxtotgroupsize = NULL,
mintotgroupsize = NULL,
xt_space = NULL,
a = NULL,
maxa = NULL,
mina = NULL,
a_space = NULL,
x_space = NULL,
use_grouped_xt = FALSE,
grouped_xt = NULL,
use_grouped_a = FALSE,
grouped_a = NULL,
use_grouped_x = FALSE,
grouped_x = NULL,
our_zero = NULL,
auto_pointer = "",
user_distribution_pointer = "",
minxt = NULL,
maxxt = NULL,
discrete_xt = NULL,
discrete_a = NULL,
fixRes = FALSE,
script = NULL,
overwrite = TRUE,
literalFix = TRUE,
opt_xt = FALSE,
opt_a = FALSE,
opt_x = FALSE,
opt_samps = FALSE,
optTime = TRUE,
...
)

```

Arguments

- | | |
|---------------|---|
| stickyRecalcN | The number of bad ODE solves before reducing the atol/rtol for the rest of the problem. |
| maxOdeRecalc | Maximum number of times to reduce the ODE tolerances and try to resolve the |

	system if there was a bad ODE solve.
odeRecalcFactor	The ODE recalculation factor when ODE solving goes bad, this is the factor the rtol/ atol is reduced
maxn	Maximum number of design points for optimization; By default this is declared by the maximum number of design points in the babelmixr2 dataset (when NULL)
rxControl	'rxode2' ODE solving options during fitting, created with 'rxControl()'
sigdig	Optimization significant digits. This controls: <ul style="list-style-type: none"> • The tolerance of the inner and outer optimization is $10^{-\text{sigdig}}$ • The tolerance of the ODE solvers is $0.5 \times 10^{-(\text{sigdig}-2)}$; For the sensitivity equations and steady-state solutions the default is $0.5 \times 10^{-(\text{sigdig}-1.5)}$ (sensitivity changes only applicable for liblsoda) • The tolerance of the boundary check is $5 \times 10^{-(\text{sigdig} + 1)}$
important	character vector of important parameters or NULL for default. This is used with Ds-optimality
unimportant	character vector of unimportant parameters or NULL for default. This is used with Ds-optimality
iFIMCalculationType	can be either an integer or a named value of the Fisher Information Matrix type: <ul style="list-style-type: none"> • 0/"full" = Full FIM • 1/"reduced" = Reduced FIM • 2/"weighted" = weighted models • 3/"loc" = Loc models • 4/"reducedPFIM" = reduced FIM with derivative of SD of sigma as in PFIM • 5/"fullABC" = FULL FIM parameterized with A,B,C matrices & derivative of variance • 6/"largeMat" = Calculate one model switch at a time, good for large matrices • 7/"reducedFIMABC" = Reduced FIM parameterized with A,B,C matrices & derivative of variance
iApproximationMethod	Approximation method for model, 0=FO, 1=FOCE, 2=FOCEI, 3=FOI
iFOCNumInd	integer; number of individuals in focei solve
prior_fim	matrix; prior FIM
d_switch	integer or character option: <ul style="list-style-type: none"> • 0/"ed" = ED design • 1/"d" = D design
ofv_calc_type	objective calculation type: <ul style="list-style-type: none"> • 1/"d" = D-optimality". Determinant of the FIM: $\det(\text{FIM})$ • 2/"a" = "A-optimality". Inverse of the sum of the expected parameter variances: $1/\text{trace_matrix}(\text{inv}(\text{FIM}))$

- 4/"lnD" = "lnD-optimality". Natural logarithm of the determinant of the FIM: $\log(\det(\text{FIM}))$
- 6/"Ds" = "Ds-optimality". Ratio of the Determinant of the FIM and the Determinant of the uninteresting rows and columns of the FIM: $\det(\text{FIM})/\det(\text{FIM}_u)$
- 7/"inverse" = Inverse of the sum of the expected parameter RSE: $1/\sum(\text{get_rse}(\text{FIM}, \text{poped.db}, \text{use_pe}))$

strEDPenaltyFile Penalty function name or path and filename, empty string means no penalty. User defined criterion can be defined this way.

ofv_fun User defined function used to compute the objective function. The function must have a poped database object as its first argument and have "..." in its argument list. Can be referenced as a function or as a file name where the function defined in the file has the same name as the file. e.g. "cost.txt" has a function named "cost" in it.

iEDCalculationType ED Integral Calculation type:

- 0/"mc" = Monte-Carlo-Integration
- 1/"laplace" = Laplace Approximation
- 2/"bfgs-laplace" = BFGS Laplace Approximation

ED_samp_size Sample size for E-family sampling

bLHS How to sample from distributions in E-family calculations. 0=Random Sampling, 1=LatinHyperCube –

bUseRandomSearch • *******START OF Optimization algorithm SPECIFICATION OPTIONS*******
Use random search (1=TRUE, 0=FALSE)

bUseStochasticGradient Use Stochastic Gradient search (1=TRUE, 0=FALSE)

bUseLineSearch Use Line search (1=TRUE, 0=FALSE)

bUseExchangeAlgorithm Use Exchange algorithm (1=TRUE, 0=FALSE)

bUseBFGSMinimizer Use BFGS Minimizer (1=TRUE, 0=FALSE)

bUseGrouped_xt Use grouped time points (1=TRUE, 0=FALSE).

EACriteria Exchange Algorithm Criteria:

- 1/"modified" = Modified
- 2/"fedorov" = Fedorov

strRunFile Filename and path, or function name, for a run file that is used instead of the regular PopED call.

poped_version • *******START OF Labeling and file names SPECIFICATION OPTIONS*******
The current PopED version

modtit The model title

output_file Filename and path of the output file during search

output_function_file Filename suffix of the result function file

strIterationFileName	Filename and path for storage of current optimal design
user_data	<ul style="list-style-type: none"> • *****START OF Miscellaneous SPECIFICATION OPTIONS***** User defined data structure that, for example could be used to send in data to the model
ourzero	Value to interpret as zero in design
dSeed	The seed number used for optimization and sampling – integer or -1 which creates a random seed as <code>.integer(Sys.time())</code> or NULL.
line_opta	Vector for line search on continuous design variables (1=TRUE,0=FALSE)
line_optx	Vector for line search on discrete design variables (1=TRUE,0=FALSE)
bShowGraphs	Use graph output during search
use_logfile	If a log file should be used (0=FALSE, 1=TRUE)
m1_switch	Method used to calculate M1: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference • 20/"analytic" = Analytic derivative • 30/"ad" = Automatic differentiation
m2_switch	Method used to calculate M2: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference • 20/"analytic" = Analytic derivative • 30/"ad" = Automatic differentiation
hle_switch	Method used to calculate linearization of residual error: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference • 30/"ad" = Automatic differentiation
gradff_switch	Method used to calculate the gradient of the model: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference • 20/"analytic" = Analytic derivative • 30/"ad" = Automatic differentiation
gradfg_switch	Method used to calculate the gradient of the parameter vector g: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference • 20/"analytic" = Analytic derivative • 30/"ad" = Automatic differentiation
grad_all_switch	Method used to calculate all the gradients: <ul style="list-style-type: none"> • 1/"central" = Central difference • 0/"complex" = Complex difference

rsit_output	Number of iterations in random search between screen output
sgit_output	Number of iterations in stochastic gradient search between screen output
hm1	Step length of derivative of linearized model w.r.t. typical values
hlf	Step length of derivative of model w.r.t. g
hlg	Step length of derivative of g w.r.t. b
hm2	Step length of derivative of variance w.r.t. typical values
hgd	Step length of derivative of OFV w.r.t. time
hle	Step length of derivative of model w.r.t. sigma
AbsTol	The absolute tolerance for the diff equation solver
RelTol	The relative tolerance for the diff equation solver
iDiffSolverMethod	The diff equation solver method, NULL as default.
bUseMemorySolver	If the differential equation results should be stored in memory (1) or not (0)
rsit	Number of Random search iterations
sgit	Number of stochastic gradient iterations
intrsit	Number of Random search iterations with discrete optimization.
intsgit	Number of Stochastic Gradient search iterations with discrete optimization
maxrsnullit	Iterations until adaptive narrowing in random search
convergence_eps	Stochastic Gradient convergence value, (difference in OFV for D-optimal, difference in gradient for ED-optimal)
rslxt	Random search locality factor for sample times
rsla	Random search locality factor for covariates
cfaxt	Stochastic Gradient search first step factor for sample times
cfaa	Stochastic Gradient search first step factor for covariates
bGreedyGroupOpt	Use greedy algorithm for group assignment optimization
EAStepSize	Exchange Algorithm StepSize
EANumPoints	Exchange Algorithm NumPoints
EAConvergenceCriteria	Exchange Algorithm Convergence Limit/Criteria
bEANoReplicates	Avoid replicate samples when using Exchange Algorithm
BFGSProjectedGradientTol	BFGS Minimizer Convergence Criteria Normalized Projected Gradient Tolerance
BFGSTolerancef	BFGS Minimizer Line Search Tolerance f
BFGSToleranceg	BFGS Minimizer Line Search Tolerance g
BFGSTolerancex	BFGS Minimizer Line Search Tolerance x

ED_diff_it	Number of iterations in ED-optimal design to calculate convergence criteria
ED_diff_percent	ED-optimal design convergence criteria in percent
line_search_it	Number of grid points in the line search
Doptim_iter	Number of iterations of full Random search and full Stochastic Gradient if line search is not used
iCompileOption	<p>Compile options for PopED</p> <ul style="list-style-type: none"> • "none"/-1 = No compilation • "full"/0 or 3 = Full compilation • "mcc"/1 or 4 = Only using MCC (shared lib) • "mpi"/2 or 5 = Only MPI, <p>When using numbers, option 0,1,2 runs PopED and option 3,4,5 stops after compilation.</p> <p>When using characters, the option compileOnly determines if the model is only compiled (and PopED is not run).</p>
compileOnly	logical; only compile the model, do not run PopED (in conjunction with iCompileOption)
iUseParallelMethod	<p>Parallel method to use</p> <ul style="list-style-type: none"> • 0/"matlab" = Matlab PCT • 1/"mpi" = MPI
MCC_Dep	Additional dependencies used in MCC compilation (mat-files), if several space separated
strExecuteName	Compilation output executable name
iNumProcesses	Number of processes to use when running in parallel (e.g. 3 = 2 workers, 1 job manager)
iNumChunkDesignEvals	Number of design evaluations that should be evaluated in each process before getting new work from job manager
Mat_Out_Pre	The prefix of the output mat file to communicate with the executable
strExtraRunOptions	Extra options send to e\$. the MPI executable or a batch script, see execute_parallel\$m for more information and options
dPollResultTime	Polling time to check if the parallel execution is finished
strFunctionInputName	The file containing the popedInput structure that should be used to evaluate the designs
bParallelRS	If the random search is going to be executed in parallel
bParallelSG	If the stochastic gradient search is going to be executed in parallel
bParallelMFEA	If the modified exchange algorithm is going to be executed in parallel
bParallelLS	If the line search is going to be executed in parallel

groupsize	Vector defining the size of the different groups (num individuals in each group). If only one number then the number will be the same in every group.
time	string that represents the time in the dataset (ie xt)
timeLow	string that represents the lower design time (ie minxt)
timeHi	string that represents the upper design time (ie maxmt)
id	The id variable
m	Number of groups in the study. Each individual in a group will have the same design.
x	A matrix defining the initial discrete values for the model Each row is a group/individual.
ni	Vector defining the number of samples for each group.
maxni	<ul style="list-style-type: none"> • *****START OF DESIGN SPACE OPTIONS***** Max number of samples per group/individual
minni	Min number of samples per group/individual
maxtotni	Number defining the maximum number of samples allowed in the experiment.
mintotni	Number defining the minimum number of samples allowed in the experiment.
maxgroupsize	Vector defining the max size of the different groups (max number of individuals in each group)
mingroupsize	Vector defining the min size of the different groups (min num individuals in each group) –
maxtotgroupsize	The total maximal groupsize over all groups
mintotgroupsize	The total minimal groupsize over all groups
xt_space	Cell array <code>cell</code> defining the discrete variables allowed for each xt value. Can also be a vector of values <code>c(1:10)</code> (same values allowed for all xt), or a list of lists <code>list(1:10, 2:23, 4:6)</code> (one for each value in xt in row major order or just for one row in xt, and all other rows will be duplicated).
a	Matrix defining the initial continuous covariate values. <code>n_rows=number of groups</code> , <code>n_cols=number of covariates</code> . If the number of rows is one and the number of groups > 1 then all groups are assigned the same values.
maxa	Vector defining the max value for each covariate. If a single value is supplied then all a values are given the same max value
mina	Vector defining the min value for each covariate. If a single value is supplied then all a values are given the same max value
a_space	Cell array <code>cell</code> defining the discrete variables allowed for each a value. Can also be a list of values <code>list(1:10)</code> (same values allowed for all a), or a list of lists <code>list(1:10, 2:23, 4:6)</code> (one for each value in a).
x_space	Cell array <code>cell</code> defining the discrete variables for each x value.
use_grouped_xt	Group sampling times between groups so that each group has the same values (TRUE or FALSE).
grouped_xt	Matrix defining the grouping of sample points. Matching integers mean that the points are matched. Allows for finer control than <code>use_grouped_xt</code>

use_grouped_a	Group continuous design variables between groups so that each group has the same values (TRUE or FALSE).
grouped_a	Matrix defining the grouping of continuous design variables. Matching integers mean that the values are matched. Allows for finer control than use_grouped_a.
use_grouped_x	Group discrete design variables between groups so that each group has the same values (TRUE or FALSE).
grouped_x	Matrix defining the grouping of discrete design variables. Matching integers mean that the values are matched. Allows for finer control than use_grouped_x.
our_zero	Value to interpret as zero in design.
auto_pointer	Filename and path, or function name, for the Autocorrelation function, empty string means no autocorrelation
user_distribution_pointer	Filename and path, or function name, for user defined distributions for E-family designs
minxt	Matrix or single value defining the minimum value for each xt sample. If a single value is supplied then all xt values are given the same minimum value
maxxt	Matrix or single value defining the maximum value for each xt sample. If a single value is supplied then all xt values are given the same maximum value.
discrete_xt	Cell array <code>cell</code> defining the discrete variables allowed for each xt value. Can also be a list of values <code>list(1:10)</code> (same values allowed for all xt), or a list of lists <code>list(1:10, 2:23, 4:6)</code> (one for each value in xt). See examples in create_design_space .
discrete_a	Cell array <code>cell</code> defining the discrete variables allowed for each a value. Can also be a list of values <code>list(1:10)</code> (same values allowed for all a), or a list of lists <code>list(1:10, 2:23, 4:6)</code> (one for each value in a). See examples in create_design_space .
fixRes	boolean; Fix the residuals to what is specified by the model
script	write a PopED/rxode2 script that can be modified for more fine control. The default is NULL. When <code>script</code> is TRUE, the script is returned as a lines that would be written to a file and with the class <code>babelmixr2popedScript</code> . This allows it to be printed as the script on screen. When <code>script</code> is a file name (with an R extension), the script is written to that file.
overwrite	<code>[logical(1)]</code> If TRUE, an existing file in place is allowed if it is both readable and writable. Default is FALSE.
literalFix	boolean, substitute fixed population values as literals and re-adjust ui and parameter estimates after optimization; Default is 'TRUE'.
opt_xt	boolean to indicate if this is meant for optimizing times
opt_a	boolean to indicate if this is meant for optimizing covariates
opt_x	boolean to indicate if the discrete design variables be optimized

opt_samps	boolean to indicate if the sample optimizer is used (not implemented yet in PopED)
optTime	boolean to indicate if the global time indexer inside of babelmixr2 is reset if the times are different. By default this is TRUE. If FALSE you can get slightly better run times and possibly slightly different results. When optTime is FALSE the global indexer is reset every time the PopED rxode2 is setup for a problem or when a poped dataset is created. You can manually reset with popedMultipleEndpointResetTimeIndex
...	other parameters for PopED control

Value

popedControl object

Author(s)

Matthew L. Fidler

popedGetMultipleEndpointModelingTimes

Get Multiple Endpoint Modeling Times

Description

This function takes a vector of times and a corresponding vector of IDs, groups the times by their IDs, initializes an internal C++ global TimeIndexer, that is used to efficiently lookup the final output from the rxode2 solve and then returns the sorted unique times.

The popedMultipleEndpointIndexDataFrame() function can be used to visualize the internal data structure inside R, but it does not show all the indexes in the case of time ties for a given ID. Rather it shows one of the indexes and the total number of indexes in the data.frame

Usage

```
popedGetMultipleEndpointModelingTimes(times, modelSwitch, sorted = FALSE)
```

```
popedMultipleEndpointIndexDataFrame(print = FALSE)
```

Arguments

times	A numeric vector of times.
modelSwitch	An integer vector of model switch indicator corresponding to the times
sorted	A boolean indicating if the returned times should be sorted
print	boolean for popedMultipleEndpointIndexDataFrame() when TRUE show each id/index per time even though it may not reflect in the returned data.frame

Value

A numeric vector of unique times.

Examples

```
times <- c(1.1, 1.2, 1.3, 2.1, 2.2, 3.1)
modelSwitch <- c(1, 1, 1, 2, 2, 3)
sortedTimes <- popedGetMultipleEndpointModelingTimes(times, modelSwitch, TRUE)
print(sortedTimes)

# now show the output of the data frame representing the model
# switch to endpoint index

popedMultipleEndpointIndexDataFrame()

# now show a more complex example with overlaps etc.

times <- c(1.1, 1.2, 1.3, 0.5, 2.2, 1.1, 0.75,0.75)
modelSwitch <- c(1, 1, 1, 2, 2, 2, 3, 3)
sortedTimes <- popedGetMultipleEndpointModelingTimes(times, modelSwitch, TRUE)
print(sortedTimes)

popedMultipleEndpointIndexDataFrame(TRUE) # Print to show individual matching
```

popedMultipleEndpointResetTimeIndex

Reset the Global Time Indexer for Multiple Endpoint Modeling

Description

This clears the memory and resets the global time indexer used for multiple endpoint modeling.

Usage

```
popedMultipleEndpointResetTimeIndex()
```

Value

NULL, called for side effects

Examples

```
popedMultipleEndpointResetTimeIndex()
```

rxToMonolix *Convert RxODE syntax to monolix syntax*

Description

Convert RxODE syntax to monolix syntax

Usage

```
rxToMonolix(x, ui)
```

Arguments

x	Expression
ui	rxode2 ui

Value

Monolix syntax

Author(s)

Matthew Fidler

rxToNonmem *Convert RxODE syntax to NONMEM syntax*

Description

Convert RxODE syntax to NONMEM syntax

Usage

```
rxToNonmem(x, ui)
```

Arguments

x	Expression
ui	rxode2 ui

Value

NONMEM syntax

Author(s)

Matthew Fidler

simplifyUnit	<i>Simplify units by removing repeated units from the numerator and denominator</i>
--------------	---

Description

Simplify units by removing repeated units from the numerator and denominator

Usage

```
simplifyUnit(numerator = "", denominator = "")
```

Arguments

numerator	The numerator of the units (or the whole unit specification)
denominator	The denominator of the units (or NULL if numerator is the whole unit specification)

Details

NA or "" for numerator and denominator are considered unitless.

Value

The units specified with units that are in both the numerator and denominator cancelled.

See Also

Other Unit conversion: [modelUnitConversion\(\)](#)

Examples

```
simplifyUnit("kg", "kg/mL")  
# units that don't match exactly are not cancelled  
simplifyUnit("kg", "g/mL")
```

Index

* Unit conversion

- modelUnitConversion, 10
- simplifyUnit, 33
- .setupPopEDdatabase, 2

- as.nlmixr (as.nlmixr2), 3
- as.nlmixr2, 3

- babel.poped.database, 5
- babelBpopIdx, 5
- bb1DatToMonolix, 7
- bb1DatToMrgsolve (bb1DatToMonolix), 7
- bb1DatToNonmem (bb1DatToMonolix), 7
- bb1DatToPknca (bb1DatToMonolix), 7
- bb1DatToRxode (bb1DatToMonolix), 7

- cell, 28, 29
- create_design_space, 29

- getStandardColNames, 10

- modelUnitConversion, 10, 33
- monolixControl, 11

- nlmixr2Est.pknca, 14
- nonmemControl, 15

- pkncaControl, 18
- popedControl, 19
- popedGetMultipleEndpointModelingTimes, 30
- popedMultipleEndpointIndexDataFrame (popedGetMultipleEndpointModelingTimes), 30
- popedMultipleEndpointResetTimeIndex, 31

- rxToMonolix, 32
- rxToNonmem, 32

- simplifyUnit, 11, 33