

# Package: kwb.demeau (via r-universe)

August 30, 2024

**Title** Heat tracer study SVH

**Version** 0.0.0.9000

**Description** Heat tracer study for SVH site using USGS VS2DH model.

**License** MIT + file LICENSE

**URL** <https://github.com/KWB-R/kwb.demeau>

**BugReports** <https://github.com/KWB-R/kwb.demeau/issues>

**Depends** R (>= 3.0.0), shapefiles, hydroGOF, lattice, latticeExtra,  
kwb.vs2dh, kwb.utils, kwb.db

**Imports** RCurl, plyr, sp

**Suggests** testthat

**Remotes** [github::kwb-r/kwb.utils](https://github.com/kwb-r/kwb.utils), [github::kwb-r/kwb.db](https://github.com/kwb-r/kwb.db),  
[github::kwb-r/kwb.vs2dh](https://github.com/kwb-r/kwb.vs2dh)

**Encoding** UTF-8

**LazyLoad** yes

**RoxygenNote** 6.1.1

**Repository** <https://kwb-r.r-universe.dev>

**RemoteUrl** <https://github.com/KWB-R/kwb.demeau>

**RemoteRef** HEAD

**RemoteSha** 3c82a60433956879b9812472fba7075dd9318bee

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---

```
addHorizontalDistances
```

*Helper function: add horizontal distances from left boundary coordinates*

---

## Description

Helper function: add horizontal distances from left boundary coordinates

## Usage

```
addHorizontalDistances(gisData, leftBoundaryRow = 1)
```

## Arguments

```
gisData      data.frame as retrieved by importShapefiles()  
leftBoundaryRow  
            row number index of "gisData" which contains the left model boundary (Default:  
            1)
```

## Value

Model coordinates instead of "real" world coordinates

## Examples

```
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")  
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)  
### Store GIS data in R data.frame "gisData"  
gisData <- importShapefiles(shp.files)  
### Add horizontal distances from left boundary and ignore all features that  
### have larger distances than "right" boundary  
gisData <- addHorizontalDistances(gisData)  
### Plot horizontal model coordinates  
maxVertical <- -abs(max(gisData$fcBottom, na.rm=TRUE))
```

---

```
calcWaterLevelChange  Helper function: calculate water level change
```

---

## Description

Helper function: calculate water level change

## Usage

```
calcWaterLevelChange(refDate = "2009-03-02", df)
```

## Arguments

refDate	reference date for start (Default: "2009-03-02")
df	data frame with structure like moniDat\$agg\$dailyMedian

calibrateModel	<i>Calibration: single parameter</i>
----------------	--------------------------------------

## Description

Calibration: single parameter

## Usage

```
calibrateModel(preparedHeatModel, moniDat, obsPoints = "*",
               parameterName = "ratioKzKh", parameterRange = c(0.01, 0.1),
               objState = "waterLevelChange", objCrit = "RMSE", ...)
```

## Arguments

preparedHeatModel	as retrieved by prepareHeatModel()
moniDat	moniDat
obsPoints	regular expression of observation points/wells to be included for goodness of fit calculation (Default: *, i.e. all); if only BSV-6_3, then: "BSV-6-3"
parameterName	parameterName (Default: "ratioKzKh")
parameterRange	parameterRange (Default: c(0.01, 0.1))
objState	model state variable to be optimised either "waterLevelChange" or "temp" (for temperature) (Default: "waterLevelChange")
objCrit	vector with performance parameters produced by function hydroGOF:gof(), Default: "RMSE" (valid parameters: "ME", "MAE", "MSE", "RMSE", "NRMSE", "PBIAS", "RSR", "rSD", "NSE", "mNSE", "rNSE", "d", "md", "rd", "cp", "r", "R2", "bR2", "KGE", "VE"), ATTENTION: currently optimising is implemented to MINIMISE the value of only ONE selected objCrit parameter. Thus please make sure that the best model fit results of the MINIMUM of the selected parameter
...	further arguments passed to hydroGOF::gof()

## Value

calibration results

---

```
compareModelledMeasured
```

*Compare measured & modelled results*

---

### Description

Compare measured & modelled results

### Usage

```
compareModelledMeasured(heatModel, moniDat, toPlot = TRUE)
```

### Arguments

heatModel	object as retrieved by runHeatModel()
moniDat	as retrieved by processingData()
toPlot	If TRUE results are plotted (Default: TRUE)

### Value

Plot/List of water level, water level change & temperature of measured vs. modelled data

---

```
convertToListAndAddMoniColumns
```

*Monitoring: convert to list & add monitoring columns*

---

### Description

Monitoring: convert to list & add monitoring columns

### Usage

```
convertToListAndAddMoniColumns(df, keyFields = "myDateTime")
```

### Arguments

df	dataframe containing the data to be transformed
keyFields	keyFields to be used as keyFields in kwb.hsMatrixToListForm (Default: "myDateTime")

`convHeadBoundary`      *Helper function: convert head boundary*

## Description

Helper function: convert head boundary

## Usage

```
convHeadBoundary(leftHead = TRUE, modelStructure, depthToWaterTable,
                 hydraulicGradient)
```

## Arguments

<code>leftHead</code>	if TRUE left head, if FALSE right head (Default: TRUE)
<code>modelStructure</code>	modelStructure as retrieved by
<code>depthToWaterTable</code>	depthToWaterTable
<code>hydraulicGradient</code>	hydraulicGradient

## Value

head boundary meta info

`convModelCoordinatesToNodes`  
*Conversion: model coordinates to nodes*

## Description

Conversion: model coordinates to nodes

## Usage

```
convModelCoordinatesToNodes(modelCoords, dx = 1, dy = 1)
```

## Arguments

<code>modelCoords</code>	as retrieved by <code>convRealToModelCoordinates()</code>
<code>dx</code>	horizontal model grid spacing (Default: 1)
<code>dy</code>	vertical model grid spacing (Default: 1)

**Value**

Model nodes corresponding to model coordinates

**Examples**

```
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)
gisData <- importShapefiles(shp.files)
### Optionally remove some features
# gisData <- removeFeatures(gisData = gisData, ignoreFeatureIDs = c(3,20))
modelCoords <- convRealToModelCoordinates(gisData, dx=1, dy=1)
modelNodes <- convModelCoordinatesToNodes(modelCoords=modelCoords)
```

---

**convRealCoordinatesToNodes**

*Conversion: "real" coordinates to model nodes*

---

**Description**

By calling functions convRealToModelCoordinates() and convModelCoordinatesToNodes()

**Usage**

```
convRealCoordinatesToNodes(gisData, dx = 1, dy = 1, y = NULL)
```

**Arguments**

gisData	data.frame() as retrieved by importShapefiles()
dx	horizontal model grid spacing (Default: 1)
dy	vertical model grid spacing (Default: 1)
y	vertical model extent (Default: NULL, i.e. maximum filter screen depth below ground level)

**Value**

model nodes

**convRealToModelCoordinates***Conversion: "real" coordinates to model coordinates***Description**

Conversion: "real" coordinates to model coordinates

**Usage**

```
convRealToModelCoordinates(gisData, dx = 1, dy = 1, y = NULL)
```

**Arguments**

gisData	data.frame() as retrieved by importShapefiles()
dx	horizontal model grid spacing (Default: 1)
dy	vertical model grid spacing (Default: 1)
y	vertical model extent (Default: NULL, i.e. maximum filter screen depth below ground level)

**Examples**

```
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)
gisData <- importShapefiles(shp.files)
### Optionally remove some features
# gisData <- removeFeatures(gisData = gisData, ignoreFeatureIDs = c(3,20))
modelCoords <- convRealToModelCoordinates(gisData, dx=1, dy=1)
xyplot(y ~ x, groups = Name, data=modelCoords, pch=16, auto.key=TRUE)
```

**defineHeadBoundary***Helper function: define head boundary***Description**

Helper function: define head boundary

**Usage**

```
defineHeadBoundary(head, nly, temp, ntx = 4, ntc = 1)
```

**Arguments**

head	as retrieved by convHeadBoundary()
nly	number of vertical nodes
temp	temperature at boundary
ntx	vector with node type identifier for boundary conditions. 0 (for no specified boundary (needed for resetting some nodes after initial recharge period); 1 (for specified pressure head); 2 (for specified flux per unit horizontal surface area in units of L/T); 3 (for possible seepage face); 4 (for specified total head); 5 (for evaporation, Note: is not implemented yet!); 6 (for specified volumetric flow in units of L3/T). 7 (for gravity drain). (The gravity drain boundary condition allows gravity driven vertical flow out of the domain assuming a unit vertical hydraulic gradient. Flow into the domain cannot occur.)"
ntc	vector with node type identifier for transport boundary conditions. 0 (for no specified boundary); 1 (for specified temperatures), (Default: 1)

**Value**

boundary head parameterisation

dominantTravelTimes     *Dominant travel time: data preprocessing*

**Description**

Dominant travel time: data preprocessing

**Usage**

```
dominantTravelTimes(concModelled, offset = 0.01)
```

**Arguments**

concModelled	as retrieved by kwb.demeau::soluteModelled()
offset	offset (Default: 0.01) used for filtering soluteModel results (i.e. maxConc/2 +- offset)

**Value**

list with dominant travel times with sublists "raw" (multiple values for each TIME\_day possible) and "agg" (median "TIME\_day" and "modelled" concentration)

**dominantTravelTimesAgg**

*Helper function for dominantTravelTimes*

---

**Description**

Helper function for dominantTravelTimes

**Usage**

```
dominantTravelTimesAgg(domTimes)
```

**Arguments**

domTimes      intermediate result of function kwb.demeau::dominantTravelTimes

**Value**

list with aggregated dominant travel times (median!)

---

**downloadMeteoData**

*Monitoring: download meteo data*

---

**Description**

Monitoring: download meteo data

**Usage**

```
downloadMeteoData(startYear = 2008, endYear = 2014)
```

**Arguments**

startYear      1.1.startYear (Default: 1.1.2008)

endYear      31.12.endYear (Default: 31.12.2014)

`filterMoniData`      *Helper function: filter monitoring data*

## Description

Helper function: filter monitoring data

## Usage

```
filterMoniData(locations = NULL, locationsCol = "moniLocation",
  paras = NULL, paraCol = "moniParName", minDate = "2009-03-02",
  maxDate = "2009-04-06", df)
```

## Arguments

locations	(Default: NULL)
locationsCol	(Default: "moniLocation")
paras	(Default: NULL)
paraCol	(Default: "moniParName")
minDate	(Default: "2009-03-02")
maxDate	(Default: "2009-04-06")
df	data.frame structure like: moniDat\$agg\$dailyMedian

`fitnessAdaptedModelConfiguration`

*Calibration: helper function "fitnessAdaptedModelConfiguration" (called by function calibrateModel())*

## Description

Calibration: helper function "fitnessAdaptedModelConfiguration" ( called by function calibrate-Model()

## Usage

```
fitnessAdaptedModelConfiguration(parameterValue, parameterName,  
    preparedHeatModel, objState = "waterLevelChange", objCrit = "RMSE",  
    moniDat, obsPoints, ...)
```

**Arguments**

parameterValue	parameterValue
parameterName	parameterName
preparedHeatModel	as retrieved by prepareHeatModel()
objState	model state variable to be optimised either "waterLevelChange" or "temp" (for temperature) (Default: "waterLevelChange")
objCrit	vector with performance parameters produced by function hydroGOF:gof(), Default: "RMSE" (valid parameters: "ME", "MAE", "MSE", "RMSE", "NRMSE", "PBIAS", "RSR", "rSD", "NSE", "mNSE", "rNSE", "d", "md", "rd", "cp", "r", "R2", "bR2", "KGE", "VE")
moniDat	moniDat
obsPoints	regular expression of observation points/wells to be included for goodness of fit calculation (Default: *, i.e. all); if only BSV-6_3, then: "BSV-6-3"
...	further arguments passed to hydroGOF::gof()

**Value**

fitness of model configuration

**fitnessWithLabel**      *Compare measured & modelled results*

**Description**

Compare measured & modelled results

**Usage**

```
fitnessWithLabel(heatModel, moniDat, objState = "waterLevelChange",
  objCrit = c("RMSE", "R2"), plotIt = TRUE, plot.type = "b",
  cex.label = 1, main = NULL, performance.in.label = TRUE, ...)
```

**Arguments**

heatModel	object as retrieved by runHeatModel()
moniDat	as retrieved by processingData()
objState	model state variable to be optimised either "waterLevelChange" or "temp" (for temperature) (Default: "waterLevelChange")
objCrit	vector with performance parameters produced by function hydroGOF:gof(), Default: "RMSE" (valid parameters: "ME", "MAE", "MSE", "RMSE", "NRMSE", "PBIAS", "RSR", "rSD", "NSE", "mNSE", "rNSE", "d", "md", "rd", "cp", "r", "R2", "bR2", "KGE", "VE")

```
plotIt      if TRUE lattice plot will be produced (Default: TRUE)
plot.type   plot type
cex.label   character expansion factor for labels
main        plot title
performance.in.label
            if TRUE, the performance indicator appears as label
...
            additional parameters passed to plot function lattice:xyplot()
```

### Value

Plot of water level, water level change & temperature of measured vs. modelled data

---

genuchten

*vanGenuchten : helper for multiple models*

---

### Description

vanGenuchten : helper for multiple models

### Usage

```
genuchten(pressureHeads = -rev(seq(0, 1000, 5)), alpha = 1, beta = 2)
```

### Arguments

```
pressureHeads  pressureHeads
alpha          alpha to be used for van Genuchten model
beta           betaa to be used for van Genuchten model
```

### Value

data.frame with columns "pressureHead, alpha, beta, effSaturation, Kr"

### References

[http://wwwbrr.cr.usgs.gov/projects/GW\\_Unsat/vs2di/hlp/solute/vanGenuchten.html](http://wwwbrr.cr.usgs.gov/projects/GW_Unsat/vs2di/hlp/solute/vanGenuchten.html)

genuchtenModel      *vanGenuchten : single model*

### Description

vanGenuchten : single model

### Usage

```
genuchtenModel(pressureHead, alpha, beta)
```

### Arguments

pressureHead	pressureHead
alpha	alpha
beta	beta

### Value

data.frame with columns "pressureHead, alpha, beta, effSaturation, Kr"

### References

[http://wwwbrr.cr.usgs.gov/projects/GW\\_Unsat/vs2di/hlp/solute/vanGenuchten.html](http://wwwbrr.cr.usgs.gov/projects/GW_Unsat/vs2di/hlp/solute/vanGenuchten.html)

genuchtenModels      *vanGenuchten : multiple models*

### Description

vanGenuchten : multiple models

### Usage

```
genuchtenModels(pressureHeads = -rev(seq(0, 6, 0.5)), alphas = seq(1,
2, 0.5), betas = 1:5)
```

### Arguments

pressureHeads	pressureHeads
alphas	vector of alphas to be used for multiple model construction
betas	vector of betas to be used for multiple model construction

### Value

data.frame with columns "pressureHead, alpha, beta, effSaturation, Kr"

**References**

[http://wwwbrr.cr.usgs.gov/projects/GW\\_Unsat/vs2di/hlp/solute/vanGenuchten.html](http://wwwbrr.cr.usgs.gov/projects/GW_Unsat/vs2di/hlp/solute/vanGenuchten.html)

getFeatures

*Helper function: Gets feature information***Description**

Aggregates gis features by shape.name & id add adds new column fid and returns additional metainformation (parameter )

**Usage**

```
getFeatures(gisData, addColNames = NULL)
```

**Arguments**

gisData	data.frame with gis features as retrieved by importShapefile(s)()
addColNames	vector with additional colnames for output data.frame (Default: NULL), for valid inputs check: colNames(gisData)

**Value**

Return the features with attributes feature id (fid), shapefile name (shape.name) and feature name (Name)

importData

*Monitoring: excel data import***Description**

Monitoring: excel data import

**Usage**

```
importData(xlsPath = NULL, metaTables = c("metadataTable",
  "commentTable"), moniTables = c("bsv4", "bsvAll", "tuberia", "inflow"),
  ignoredParNames = c("Temp_graphics_C", "DiverBaro_graphFictive_cm",
  "DiverBaro_cm"))
```

**Arguments**

<code>xlsPath</code>	full path to excel file <code>http://192.168.22.12/svn/kwb/DEMEAU/Work Areas/WA1 MAR/TracerSVH/datosTOT_StVicen+_jun2008-abr2009OK.xls</code> , if FALSE already imported data object <code>moniDat</code> is loaded (Default: NULL)
<code>metaTables</code>	vector with names of tables with meta information (Default: "metadataTable", "commentTable")
<code>moniTables</code>	vector with names of tables with monitoring data to be imported (Default: "bsv4", "bsvAll", "tuberia", "inflow")
<code>ignoredParNames</code>	vector of parNames that are ignored for storing (Default: Temp_graphics_C, DiverBaro_graphFictive_cm, DiverBaro_cm: syntetical or calculated parameters!)

**Examples**

```
#### xlsDir needs to be set correctly !!!!!
xlsDir <- "C:/Users/mrustl/Documents/WC_Server/DEMEAU/Work Areas/WA1 MAR/TracerSVH"
xlsFile <- "datosTOT_StVicen_jun2008-abr2009OK.xls"
xlsPath <- file.path(xlsDir, xlsFile)
##importData(xlsPath=xlsPath)

#### Loading with stored moniDat.RData object
#importData()
```

**importShapefile**      *GIS: imports shapefiles & dbf*

**Description**

**GIS:** imports shapefiles & dbf

**Usage**

```
importShapefile(shp.path)
```

**Arguments**

<code>shp.path</code>	full path to file (with or without file extension ".shp")
-----------------------	-----------------------------------------------------------

**Value**

Imported GIS shapefile as R data.frame

**importShapefiles**      *GIS: imports shapefiles & dbf*

### Description

GIS: imports shapefiles & dbf

### Usage

```
importShapefiles(shp.files = dir(path = system.file("extdata", "qgis",
  package = "kwb.demeau"), pattern = ".shp", full.names = TRUE))
```

### Arguments

**shp.files**      vector with full paths to shapefiles "Boundary", "Ponds", "Observation wells" to be imported (with or without file extension ".shp")

### Value

Imported GIS shapefiles in an R data.frame

### Examples

```
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)
### Store GIS data in R data.frame "gisData"
gisData <- importShapefiles(shp.files)
### Plot imported GIS data:
```

**leftBoundaryInPolygon**      *Helper function: check whether left model boundary lies within polygon*

### Description

Helper function: check whether left model boundary lies within polygon

### Usage

```
leftBoundaryInPolygon(gisData, leftBoundaryRow = 1)
```

### Arguments

**gisData**      data.frame as retrieved by importShapefiles()  
**leftBoundaryRow**      row number index of "gisData" which contains the left

---

**listToMatrixForm**      *Monitoring: convert data to matrix forma*

---

### Description

Monitoring: convert data to matrix forma

### Usage

```
listToMatrixForm(df)
```

### Arguments

**df**                  data frame with structure like: moniDat\$agg\$dailyMedian

---

**mainLabel**                  *Helper function for main label of comparision plot*

---

### Description

Helper function for main label of comparision plot

### Usage

```
mainLabel(model)
```

### Arguments

**model**                  object as retrieved by runHeatModel()

### Value

main label

---

<code>modelConfiguration</code>	<i>Model: prepare model configuration</i>
---------------------------------	-------------------------------------------

---

## Description

Model: prepare model configuration

## Usage

```
modelConfiguration(modelStructure, pondTemp = 20, gwTempIni = 12,
infRate = 0.03, depthToWaterTable = 6, hydraulicGradient = 0.001,
bnd = list(tmp = gwTempIni, ntx = 4, ntc = 1),
hk = kwb.vs2dh::vs2dh.ConfigureGenuchten(ratioKzKh = 1, ss = 0, satKh =
750, porosity = 0.2, alpha = 2.3, rmc = 0, beta = 5.8),
ht = kwb.vs2dh::vs2dh.ConfigureTrans(), iniOutputTime = 1/(3600 *
24), minSimTime = 0.5, maxSimTime = 31, outputTimeStep = 1,
solver = kwb.vs2dh::vs2dh.ConfigureBasicSolver(),
rSolver = kwb.vs2dh::vs2dh.ConfigureRechargePeriodSolver())
```

## Arguments

<code>modelStructure</code>	as retrieved by convRealCoordinatesToNodes()
<code>pondTemp</code>	constant pond temperature (default: 20)
<code>gwTempIni</code>	initial groundwater temperature (default: 12)
<code>infRate</code>	infiltration rate per unit area (Default: 0.9514151 m/d)
<code>depthToWaterTable</code>	water table below ground level (default: 6 m)
<code>hydraulicGradient</code>	hydraulic gradient between left & right model boundary (Default: 0), if positive flow is from left to right, if negative from right to left
<code>bnd</code>	list of structure list(temp=VALUE, ntx=VALUE, ntc=VALUE) passed to function defineHeadBoundary (i.e. boundary with seepage face), if bnd=NULL left/right boundaries are no-flow boundaries
<code>hk</code>	hydraulic properties of soil as retrieved by kwb.vs2dh::vs2dh.ConfigureGenuchten()
<code>ht</code>	transport properties of soil as retrieved by kwb.vs2dh::vs2dh.ConfigureTrans()
<code>iniOutputTime</code>	automatically output results after 1 second of simulation
<code>minSimTime</code>	minimum simulation time in days (default: 0.5)
<code>maxSimTime</code>	maximum simulation time in days (default: 31)
<code>outputTimeStep</code>	at which timestep are the results printed (default: 1 ), i.e. each day
<code>solver</code>	general solver (Default: kwb.vs2dh::vs2dh.ConfigureBasicSolver())
<code>rSolver</code>	recharge period solver (Default: kwb.vs2dh::vs2dh.ConfigureRechargePeriodSolver())

**Value**

SVH model configuration

**See Also**

`defineHeadBoundary` for valid additional arguments

**Examples**

```
## Not run:
#### Importing GIS features
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)
gisData <- importShapefiles(shp.files)

#### Optionally remove some features
gisData <- removeFeatures(gisData = gisData, ignoreFeatureIDs = c(3,20))
modelStructure <- convRealCoordinatesToNodes(gisData = gisData)

#### Model config
conf <- modelConfiguration(modelStructure = modelStructure)

#### Running the configuration in VS2DH
res <- kwb.vs2dh::vs2di.runConfig(conf = conf, openTargetDir = TRUE)

#### Plotting results
kwb.vs2dh::vs2dh.plotObservationPoints(
  paras = "TEMP", paraLabel = "Temperature", data = res$obsPoints
)
kwb.vs2dh::vs2dh.plotVariables(para = "Temp", data = res$variables)

## End(Not run)
```

**modelCoordinatesToFeature**

*Conversion: feature parameterisation*

**Description**

Conversion: feature parameterisation

**Usage**

```
modelCoordinatesToFeature(x = c(100, 220), y = 0, dx = 0.5,
  dy = 0.5, pondDepth = verticalCmToMeters(cm = 1.2), steepness = 45)
```

**Arguments**

x	absolute horizontal min/max coordinates of model feature. L, Default: c(100,220)
y	absolute vertical min/max coordinates of model feature. L, Default: c(0,0)
dx	dx
dy	dy
pondDepth	Depth of pond below ground level (Default: verticalCmToMeters(cm = 1.2), i.e. 3.4m, derived from Figure 8, p.11 ENSAT report)
steepness	of pond bank (in degree) only used for ponds if "pondDepth" is defined (Default: 45 degree)

**Value**

Parameterisation of model features

modelFitness

*Calibration: helper function "modelFitness" (called by function modelFitnessAggregated())*

**Description**

Calibration: helper function "modelFitness" (called by function modelFitnessAggregated())

**Usage**

```
modelFitness(modelledMeasured, obsPoints = "*", ...)
```

**Arguments**

modelledMeasured	as retrieved by compareModelledMeasured() either \$temp or \$waterLevelChange
obsPoints	regular expression of observation points/wells to be included for goodness of fit calculation (Default: *, i.e. all); if only BSV-6_3, then: "BSV-6-3"
...	further arguments passed to hydroGOF::gof()

**Value**

matrix with goodness of fit criteria

`modelFitnessAggregated`

*Calibration: helper function "modelFitnessAggregated" (called by function fitnessAdaptedModelConfiguration())*

## Description

Calibration: helper function "modelFitnessAggregated" (called by function fitnessAdaptedModelConfiguration())

## Usage

```
modelFitnessAggregated(modelledMeasured, obsPoints = "*",  
objCrit = "RMSE", ...)
```

## Arguments

<code>modelledMeasured</code>	as retrieved by compareModelledMeasured() either \$temp or \$waterLevelChange
<code>obsPoints</code>	regular expression of observation points/wells to be included for goodness of fit calculation (Default: *, i.e. all); if only BSV-6_3, then: "BSV-6-3"
<code>objCrit</code>	vector with performance parameters produced by function hydroGOF:gof(), Default: "RMSE" (valid parameters: "ME", "MAE", "MSE", "RMSE", "NRMSE", "PBIAS", "RSR", "rSD", "NSE", "mNSE", "rNSE", "d", "md", "rd", "cp", "r", "R2", "bR2", "KGE", "VE")
<code>...</code>	further arguments passed to hydroGOF::gof()

## Value

matrix with goodness of fit criteria

`nodeIdToRowColumn`

*Helper function: converting node ID to row/column*

## Description

Helper function: converting node ID to row/column

## Usage

```
nodeIdToRowColumn(nodeID, numberOfRows)
```

## Arguments

<code>nodeID</code>	vector of node ids
<code>numberOfRows</code>	number of rows (here: nly)

**Value**

row (yNode) and column of node ID in grid

orderedDataFrame

*Helper function to order data frame by two columns (col1, col2)*

**Description**

Helper function to order data frame by two columns (col1, col2)

**Usage**

```
orderedDataFrame(df, col1 = "Name", col2 = "TIME_day")
```

**Arguments**

df	data.frame
col1	first column to be used for ordering (Default: Name)
col2	second column to be used for ordering (Default: TIME_day)
...	further arguments passed to function order(), e.g. decreasing = TRUE

**Value**

ordered (default: ascending) data.frame according to col1 & col2

plotGenuchtenModels

*vanGenuchten : plot models*

**Description**

vanGenuchten : plot models

**Usage**

```
plotGenuchtenModels(models = genuchtenModels(), ...)
```

**Arguments**

models	as retrieved by genuchtenModels()
...	further arguments passed to lattice::xyplot()

**Value**

plot of all genuchten models

`plotModelStructure`      *Plot model Structure*

### Description

Plot model Structure

### Usage

```
plotModelStructure(df, xColName = "x", yColName = "y")
```

### Arguments

<code>df</code>	data.frame as retrieved by convRealToModelCoordinates() or convModelCoordinatesToNodes()
<code>xColName</code>	name of x column to plot
<code>yColName</code>	name of y column to plot

`plotMonitoringData`      *Monitoring: plot data*

### Description

Monitoring: plot data

### Usage

```
plotMonitoringData(moniParName = "WaterLevel_cm",
                   moniLocationPattern = "BSV|Tuberia", minDate = "2000-01-01",
                   maxDate = "2015-01-01", groups = FALSE, df)
```

### Arguments

<code>moniParName</code>	(Default: "WaterLevel_cm")
<code>moniLocationPattern</code>	(Default: "BSV Tuberia")
<code>minDate</code>	(Default: "2000-01-01")
<code>maxDate</code>	(Default: "2015-01-01")
<code>groups</code>	(Default: FALSE)
<code>df</code>	data frame

---

plotMonitoringWithTwoYAxes*Monitoring: plot data with two y axex*

---

**Description**

Monitoring: plot data with two y axex

**Usage**

```
plotMonitoringWithTwoYAxes(parY1 = "WaterLevelChange_cm",
  parY2 = "Temp_C", labelParY1 = "Water level change (cm)",
  labelParY2 = "Temperature (C)", df, ...)
```

**Arguments**

parY1	name of parameter for Y1 axis (see: colnames(listToMatrixForm(df)), (Default: "WaterLevelChange_cm")
parY2	name of parameter for Y2 axis (see: colnames(listToMatrixForm(df)), (Default: "Temp_C")
labelParY1	user defined label for Y1 for legend (Default: "Water level change (cm)")
labelParY2	user defined label for Y2 for legend (Default: "Temperature (degree C)")
df	data.frame with structure like moniDat\$agg\$dailyMedian
...	further parameters passed to xyplot()

---

prepareModel*Prepare model: wrapper for modelConfiguration()*

---

**Description**

Prepare model: wrapper for modelConfiguration()

**Usage**

```
prepareModel(gisData, type = "heat", rech_pondInfRate = 1,
  rech_pondTemp = 13.7, rech_pondConc = 1, init_gwTemp = 19,
  init_gwConc = 0, init_depthToWaterTable = 6, init_hydrGrad = 0.001,
  grid_dx = 1, grid_dy = 1, grid_yMax = NULL,
  flow_ratioKzKh = 0.01, flow_satKh = 450, flow_ss = 0,
  flow_neff = 0.2, flow_rmc = 0.05, flow_alpha = 2, flow_beta = 5,
  heat_alphaL = 1, heat_alphaT = 0.1, heat_cs = 2180000,
  heat_ktRmc = 129600, heat_ktSat = 155520, heat_cw = 4180000,
  solu_alphaL = 1, solu_alphaT = 0.1, solu_molDiffCoeff = 4.5e-05 *
  3600 * 24/100, solu_decayConst = 0, solu_bulkDensity = 0,
```

```

solu_adsorp = 0, time_firstOutput = 1/(3600 * 24),
time_minSimTime = 0.5, time_maxSimTime = 30.5,
time_outputTimeStep = 1, solv_cis = TRUE, solv_cit = TRUE,
solv_numt = 5000, solv_minit = 2, solv_itmax = 300,
solv_eps = 0.001, solv_eps1 = 0.001, solv_eps2 = 0.001,
solv_hmax = 0.7, solv_itstop = FALSE, solr_delt = 1e-06,
solr_tmlt = 1.2, solr_dltmx = 1, solr_dltmin = 1e-06,
solr_tred = 0.5, solr_dsmax = 10, solr_sterr = 0, solr_pond = 0)

```

## Arguments

gisData	as retrieved by kwb.demeau::importShapefiles()
type	either "heat" (for heat model VS2DH) or "solute" (for solute transport model VS2DT), Default: "heat"
rech_pondInfRate	recharge rate of infiltration pond during model simulation in meter / day (Default: 1 m/d)
rech_pondTemp	median pond temperature during recharge period (Default: 13.7 C during whole simulation time, i.e. 30 days)
rech_pondConc	median substance concentration in pond during recharge period (Default: 1 during whole simulation time, i.e. 30 days)
init_gwTemp	initial groundwater temperature before infiltration (Default: 19 C)
init_gwConc	initial substance concentration in GW before infiltration (Default: 0)
init_depthToWaterTable	initial depth to groundwater table (Default: 6 m, assumption, no data)
init_hydrGrad	hydraulic gradient between left & right model boundary, if positive flow is from left to right, if negative from right to left (Default: 0.001)
grid_dx	model grid spacing in horizontal direction (Default: 1 m),
grid_dy	model grid spacing in vertical direction (Default: 1 m),
grid_yMax	maximum vertical model extent in meters (Default: NULL, i.e. maximum filter screen depth below ground level is set as maximum vertical model extent)
flow_ratioKzKh	Ratio of hydraulic conductivity in the z-coordinate direction to that in the x-coordinate direction (Default: 0.01)
flow_satKh	saturated hydraulic conductivity (Default: 450 m / day),
flow_ss	Specific storage (Ss), L^-1. (Default: 0)
flow_neff	effective porosity (Default: 0.2), sum of effective porosity and residual moisture content (rmc) are equal to parameter "porosity" used for van Genuchten model
flow_rmc	residual moisture content (Default: 0.05), sum of effective porosity and residual moisture content (rmc) are equal to parameter "porosity" used for van Genuchten model
flow_alpha	van Genuchten alpha. NOTE: alpha is as defined by van Genuchten (1980) and is the negative reciprocal of alpha' used in earlier versions (prior to version 3.0) of VS2DT, L. (Default: 2)

flow_beta	van Genuchten parameter, beta' in Healy (1990) and Lappala and others (1987), (Default: 5)
heat_alphaL	Longitudinal dispersion (Default: 1 m),
heat_alphaT	Transversal dispersion (Default: 0.1 m)
heat_cs	Heat capacity of dry solids (Cs), Q/L3 C. (Default: 2180000.0 J/m3C)
heat_ktRmc	Thermal conductivity of water sediment at residual moisture content, Q/LTC. (Default: 129600)
heat_ktSat	Thermal conductivity of water sediments at full saturation, Q/LC. (Default: 155520)
heat_cw	Heat capacity of water (Cw), which is the product of density times specific heat of water, Q/L3 C. (default: 4180000.0)
solu_alphaL	Longitudinal dispersion (Default: 1 m),
solu_alphaT	Transversal dispersion (Default: 0.1 m)
solu_molDiffCoeff	Molecular diffusion coefficient, Dm, L2/T. (Default: ( 4.5e-05*3600*24/100 m2/day, ### <a href="http://en.wikipedia.org/wiki/Mass_diffusivity#Liquids">http://en.wikipedia.org/wiki/Mass_diffusivity#Liquids</a> for hydrogen - water at 25 C)
solu_decayConst	Decay constant, l, T-1. (Default: 0)
solu_bulkDensity	Bulk density, Dm (set to 0 for no adsorption or ion exchange) M/L3. (Default: 0)
solu_adsorp	0 for no adsorption or ion exchange; Kd for linear adsorption isotherm; K1 for Langmuir isotherm; Kf for Freundlich isotherm; or Km for ion exchange. (Default: 0)
time_firstOutput	first output after x time (default: after 1 second), (-> proxy for initial setting)
time_minSimTime	start of regular output (Default: after 0.5 days)
time_maxSimTime	end of regular output & model simulation (Default: 30.5 days)
time_outputTimeStep	time interval in days for which model results are written to output file (Default: 1 day)
solv_cis	If TRUE spatial discretisation is realised by centered-in-space differencing; if FALSE backward-in-space differencing is to be used for transport equation. (default: TRUE)
solv_cit	If TRUE temporal discretisation is realised by centered-in-time differencing; if FALSE backward-in-time or fully implicit differencing is to be used. (default: TRUE)
solv_numt	Maximum number of time steps.(default: 5000). (NOTE: if enhanced precision in print out to file "balance.out" and file 11 "obsPoints.out", is desired set NUMT equal to a negative number. That is, multiply actual maximum number of time steps by -1)

solv_minit	Minimum number of iterations per time step. (default: 2)
solv_itmax	Maximum number of iterations per time step. (default: 300)
solv_eps	Head closure criterion for iterative solution of flow equation, L. (default: 0.001)
solv_eps1	Temperature closure criterion for iterative solution of transport equation, C. (default: 0.001)
solv_eps2	Velocity closure criterion for outer iteration loop at each time step, L/T. (default: 0.001)
solv_hmax	Relaxation parameter for iterative solution. See discussion in Lappala and others (1987) for more detail. Value is generally in the range of 0.4 to 1.2. (default: 0.7)
solv_itstop	If TRUE simulation is terminated after ITMAX iterations in one time step; otherwise = F. (default: FALSE)
solr_delt	Length of initial time step for this period, T. (default: 1.0E-6)
solr_tm1t	Multiplier for time step length. (default: 1.2)
solr_dltmx	Maximum allowed length of time step, T. (default: 1)
solr_dltmin	Minimum allowed length of time step, T. (default: 1.0E-6)
solr_tred	Factor by which time-step length is reduced if convergence is not obtained in IT-MAX iterations. Values usually should be in the range 0.1 to 0.5. If no reduction of time-step length is desired, input a value of 0.0. (default: 0.1)
solr_dsmax	Maximum allowed change in head per time step for this period, L. (default: 10)
solr_sterr	Steady-state head criterion; when the maximum change in head between successive time steps is less than STERR, the program assumes that steady state has been reached for this period and advances to next recharge period, L. (default: 0)
solr_pond	Maximum allowed height of ponded water for constant flux nodes. See Lappala and other (1987) for detailed discussion of POND, L. (default: 0)

### Value

Prepared SVH model configuration

### Examples

```
### Importing GIS features
shp.dir <- system.file("extdata", "qgis", package="kwb.demeau")
shp.files <- dir(path = shp.dir, pattern = ".shp", full.names = TRUE)
gisData <- importShapefiles(shp.files)
### Optionally remove some features
gisData <- removeFeatures(gisData = gisData, ignoreFeatureIDs = 20)
#### 1) Prepare heat
preparedHeatModel <- prepareModel(gisData = gisData, type = "heat")
#' #### 1) Prepare solute transport model
preparedSoluteModel <- prepareModel(gisData = gisData, type = "solu")
```

---

processingData	<i>Processing: data preprocessing</i>
----------------	---------------------------------------

---

## Description

Processing: data preprocessing

## Usage

```
processingData(rawData)
```

## Arguments

rawData	raw data imported with importData()
---------	-------------------------------------

---

removeFeatures	<i>Helper function: remove features which should be ignored</i>
----------------	-----------------------------------------------------------------

---

## Description

Helper function: remove features which should be ignored

## Usage

```
removeFeatures(gisData, ignoreFeatureIDs = NULL)
```

## Arguments

gisData	data.frame with gis features as retrieved by importShapefile(s)()
ignoreFeatureIDs	should be a valid feature id column gisData\$fID, for possible values check: unique(gisData\$fID)

## Value

input gisData (possibly removed by ignoreFeatureIDs)

`removeFileExtension`    *Helper function: removes file extensions (copied from "kwb.quantum" package)*

### Description

Helper function: removes file extensions (copied from "kwb.quantum" package)

### Usage

```
removeFileExtension(x)
```

### Arguments

<code>x</code>	file.path
----------------	-----------

### Value

file path without extension (i.e. without ".")

`renameValues`    *Helper function: rename values*

### Description

Helper function: rename values

### Usage

```
renameValues(df, colName, oldVal, newVal)
```

### Arguments

<code>df</code>	data.frame to be modified
<code>colName</code>	colName containing the values to be changed
<code>oldVal</code>	old value
<code>newVal</code>	new value

---

`runHeatModel`

*Run heat model: wrapper for vs2di.runConfig()*

---

## Description

Run heat model: wrapper for vs2di.runConfig()

## Usage

```
runHeatModel(preparedHeatModel, tDir = tempdir(),  
             openTargetDir = FALSE, ...)
```

## Arguments

preparedHeatModel	prepared heat model as retrieved by prepareModel(type="heat")
tDir	target directory where vs2dh model input/output files should be stored. (Default: tempdir())
openTargetDir	If TRUE: model directory with heat model results will be opened in Windows explorer (Default: FALSE)
...	additional arguments passed to function kwb.vs2dh::vs2di.runConfig()

## Value

List with heat model results (\$res) and configuration

---

`runSoluteModel`

*Run solute transport model: wrapper for vs2di.runConfig()*

---

## Description

Run solute transport model: wrapper for vs2di.runConfig()

## Usage

```
runSoluteModel(preparedSoluteModel, tDir = tempdir(),  
               returnOutput = TRUE, openTargetDir = FALSE, ...)
```

**Arguments**

<code>preparedSoluteModel</code>	prepared solute transport model as retrieved by <code>prepareModel(type="solu")</code>
<code>tDir</code>	target directory where vs2dh model input/output files should be stored. (Default: <code>tempdir()</code> )
<code>returnOutput</code>	Default: TRUE
<code>openTargetDir</code>	If TRUE: model directory with heat model results will be opened in Windows explorer (Default: FALSE)
<code>...</code>	additional arguments passed to function <code>kwb.vs2dh::vs2di.runConfig()</code>

**Value**

List with heat model results (\$res) and configuration

<code>selectModelled</code>	<i>Compare measured &amp; modelled results</i>
-----------------------------	------------------------------------------------

**Description**

Compare measured & modelled results

**Usage**

```
selectModelled(modDf, parName = "TEMP", func = stats::median)
```

**Arguments**

<code>modDf</code>	modDf
<code>parName</code>	(Default: "TEMP")
<code>func</code>	(Default: <code>median</code> )

**Value**

Plot of water level, water level change & temperature of measured vs. modelled data

---

`setFeatureIDs`

*Helper function: Defines feature ids for gis objects*

---

### Description

Aggregates gis features by shape.name & id add adds new column fID

### Usage

```
setFeatureIDs(x)
```

### Arguments

x data.frame with gis features as retrieved by importShapefile()

### Value

input data.frame and new column feature id (fID)

---

`setSoilZero`

*Helper function: set soil ITEX to zero*

---

### Description

Helper function: set soil ITEX to zero

### Usage

```
setSoilZero(nodes, soilGrid, shape.name = "Ponds")
```

### Arguments

nodes	as retrieved by convModelCoordinatesToNodes() or convRealCoordinatesToNodes()
soilGrid	soil grid (as retrieved by kwb.vs2dh::vs2dh.ConfigureSoilGrid())
shape.name	name of polygon shape files with ponds (Default: "Ponds")

### Value

soil grid (with possible ITEX values set to zero)

soluteModelled	<i>Compare measured &amp; modelled results</i>
----------------	------------------------------------------------

### Description

Compare measured & modelled results

### Usage

```
soluteModelled(soluteModel, offset = 0.01, toPlot = TRUE, ...)
```

### Arguments

soluteModel	object as retrieved by runSoluteModel()
offset	offset (Default: 0.01) used for filtering soluteModel results (i.e. maxConc/2 +- offset)
toPlot	If TRUE results are plotted (Default: TRUE)
...	additional parameters passed to plot function lattice:xyplot()

### Value

Plot/List of water level, water level change & temperature of measured vs. modelled data

verticalCmToMeters	<i>Helper function: converting vertical scale into meters (Figure. 08, page 11, ENSAT report)</i>
--------------------	---------------------------------------------------------------------------------------------------

### Description

Helper function: converting vertical scale into meters (Figure. 08, page 11, ENSAT report)

### Usage

```
verticalCmToMeters(cm)
```

### Arguments

cm	measured centimeters in Figure 8
----	----------------------------------

### Value

vertical length in meters

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