Package: DielectricWaterR (via r-universe)

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Title Auditing and Exploring Dielectric Measurements of Water

Version 0.2.0

Description Imports, audits, compares and visualises dielectric measurements of water under fuel contamination and ageing. Provides descriptive summaries, frequency-response comparisons, confidence intervals based on physical-unit means, and training and testing splits that keep observations from the same experimental unit together. Experimental-unit safeguards address pseudoreplication concerns discussed by Hurlbert (1984) <doi:10.2307/1942661>. Grouped splitting is consistent with the structured-data validation principles discussed by Roberts et al. (2017) <doi:10.1111/ecog.02881>. Student t confidence intervals use the standard mean-interval formula described in the NIST/SEMATECH e-Handbook of Statistical Methods <https://www.itl.nist.gov/div898/handbook/eda/section3/eda352.htm>. Experimental-unit identifiers are supplied by the user and are not inferred from material labels. This research prototype does not provide validated contaminant prediction or causal inference.

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`analyse_ageing_trajectories` *Analyse descriptive dielectric ageing trajectories*

Description

Summarises dielectric responses across ageing times at a fixed frequency and within the same material. Does not assume repeated measurements of one physical sample.

Usage

```
analyse_ageing_trajectories(
  data,
  outcome = "permittivity",
  frequency_hz,
  material = NULL
)
```

Arguments

`data`	Dielectric measurement data frame.
`outcome`	Numeric dielectric response column.
`frequency_hz`	Frequency to analyse.
`material`	Optional material label to select.

Value

Data frame containing ageing time, mean response, number of measurements and descriptive changes.

`analyse_frequency_response`

Summarise dielectric frequency responses

Description

Provides descriptive summaries of dielectric measurements across experimental conditions and frequencies. Rows with unverified or conflicting water-medium labels are excluded from the primary analysis. No independent-sample inference is performed.

Usage

```
analyse_frequency_response(data, min_frequencies = 5L)
```

Arguments

`data`	A dielectric dataset returned by read_dielectric().
`min_frequencies`	Minimum distinct frequencies per curve.

Value

A tibble containing descriptive curve summaries.

audit_dielectric *Audit dielectric data without inventing physical sample IDs*

Description

Audit dielectric data without inventing physical sample IDs

Usage

```
audit_dielectric(data)
```

Arguments

data	Output from read_dielectric().

Value

List containing summary, missingness, ranges, duplicated keys and warnings.

audit_experimental_units *Audit experimental-unit information*

Description

Summarises measurements by material label and reports whether physical sample identities can be established. Material names are not assumed to identify physical samples.

Usage

```
audit_experimental_units(data, sample_id = NULL)
```

Arguments

data	A dielectric measurement data frame.
sample_id	Optional column name containing genuine physical sample identifiers.

Value

A data frame summarising material labels, ageing times, frequencies and sample identity status.

Examples

```
# Synthetic demonstration; not experimental observations.
x <- data.frame(
  material = rep(c('Water A', 'Water B'), each = 2),
  age_hours = c(0, 0, 0, 0),
  frequency_hz = c(10, 100, 10, 100),
  sample_id = c('A1', 'A1', 'B1', 'B1')
)

audit_experimental_units(x)
audit_experimental_units(x, sample_id = 'sample_id')
```

---

audit_frequency_exclusions *Audit observation exclusions for frequency-response analysis*

Description

Classifies every observation according to its eligibility for the primary descriptive frequency-response analysis. Material-label agreement is a coding-consistency check, not independent verification of the experimental medium.

Usage

```
audit_frequency_exclusions(data)
```

Arguments

data	A dielectric dataset returned by read_dielectric().

Value

A data frame containing the original observations, their row identifiers, expected water codes, medium-label status, and analysis inclusion decisions.

---

compare_ageing *Compare dielectric measurements at two ageing times*

Description

Matches measurements by fuel, water medium, concentration and frequency. Returns descriptive ratios between two ageing times. Ratios do not establish causal effects.

Usage

```
compare_ageing(data, age_start, age_end)
```

Arguments

`data`	A dielectric measurement data frame.
`age_start`	Starting ageing time in hours.
`age_end`	Ending ageing time in hours.

Value

A data frame containing matched measurements and ratios for permittivity, dissipation factor and impedance.

`compare_common_frequency_curves` *Compare dielectric curves at exactly shared frequencies*

Description

Uses only frequencies observed in every material-age group. Does not interpolate, extrapolate, or infer sample identity. At least two shared frequencies are required for AUC.

Usage

```
compare_common_frequency_curves(data, outcome = "permittivity")
```

Arguments

`data`	Dielectric measurement data frame.
`outcome`	Numeric response column name.

Value

A list with shared frequencies, aligned responses, and curve-level AUC summaries when possible.

`compare_dielectric_fingerprints` *Compare Matched Dielectric Fingerprints*

Description

Compare petrol and diesel at identical experimental conditions using descriptive response ratios.

Usage

```
compare_dielectric_fingerprints(
  data,
  response = "permittivity",
  age_hours = 0,
  max_concentration = 20,
  exclude_conflicts = TRUE
)
```

Arguments

data	Data returned by read_dielectric().
response	One of permittivity, dissipation_factor, or impedance.
age_hours	Measurement age in hours.
max_concentration	Maximum concentration percentage.
exclude_conflicts	Exclude water-code mismatches.

Value

A list containing matched results, summary, and duplicate-condition diagnostics.

---

estimate_dielectric_ci

Estimate confidence intervals using independent physical units

---

Description

Computes a Student t confidence interval for the mean response at a single experimental condition and frequency. Multiple measurements from one physical unit are averaged first. Physical sample identifiers must be externally verified.

Usage

```
estimate_dielectric_ci(
  data,
  outcome = "permittivity",
  sample_id,
  conf_level = 0.95
)
```

Arguments

`data`	A data frame containing dielectric measurements.
`outcome`	Numeric outcome column name.
`sample_id`	Column identifying independent physical units.
`conf_level`	Confidence level between zero and one.

Value

One-row data frame containing the mean, interval, and number of independent physical units.

`evaluate_external_predictions` *Evaluate regression predictions*

Description

Calculates descriptive prediction errors. Does not establish external-data independence.

Usage

```
evaluate_external_predictions(observed, predicted)
```

Arguments

`observed`	Numeric observed responses.
`predicted`	Numeric predicted responses.

Value

One-row data frame with n, MAE, RMSE and bias.

`plot_fingerprints` *Plot dielectric frequency-response curves*

Description

Produces descriptive frequency-response curves by material and recorded ageing time. Curves do not establish independent physical replication or causal effects.

Usage

```
plot_fingerprints(
  data,
  response = "permittivity",
  title = "Descriptive dielectric frequency-response curves",
 subtitle = "Descriptive measurements; experimental independence must be verified",
  show_legend = TRUE
)
```

Arguments

data	Data frame containing dielectric measurements.
response	One of permittivity, dissipation_factor, impedance.
title	Optional plot title.
subtitle	Optional plot subtitle.
show_legend	Whether to display material and ageing legends.

Value

A ggplot object.

Examples

```
# Fully synthetic values, not experimental observations.
x <- expand.grid(
  material = c('Water A', 'Water B'),
  age_hours = c(0, 24),
  frequency_hz = c(10, 100, 1000, 10000)
)
x$permittivity <- 80 -
  4 * log10(x$frequency_hz) -
  0.1 * x$age_hours -
  ifelse(x$material == 'Water B', 3, 0)

plot_fingerprints(
  x,
  response = 'permittivity',
  title = 'Synthetic dielectric responses',
  subtitle = 'Illustrative data only'
)
```

---

read_dielectric *Import dielectric measurements from an Excel workbook*

Description

Supports standard column names, explicit header mappings, and the two original positional worksheet layouts. No experimental classifications or physical sample IDs are inferred.

Usage

```
read_dielectric(
  path,
  sheet = NULL,
  column_map = NULL,
  layout = c("auto", "standard", "legacy")
)
```

Arguments

path	Path to an Excel workbook.
sheet	Worksheet name or index. NULL selects All extract_mean when present, otherwise the first worksheet.
column_map	Named character vector mapping standard column names to workbook headers, for example c(frequency_hz = 'Frequency', permittivity = 'Epsilon').
layout	One of auto, standard, or legacy. Auto first accepts standard headers, then falls back to known legacy sheet layouts.

Details

Standard imports require material, age_hours, frequency_hz, permittivity, dissipation_factor, and impedance. Optional columns include fuel, water, concentration_pct and sample_id. Additional columns are retained in standard imports. Frequencies must already be expressed in Hz and ages in hours; renaming columns does not convert units. Analysis functions may require additional classification columns. The COded legacy layout does not supply fuel or water labels.

Value

A data frame with standardised column names.

Examples

```
path <- system.file('extdata', 'synthetic_import.xlsx',
                    package = 'DielectricWaterR')
x <- read_dielectric(path, sheet = 'Measurements', layout = 'standard')
head(x)
```

---

split_by_experimental_unit

Split measurements by verified experimental unit

Description

Keeps every observation belonging to the same physical experimental unit in either training or testing data. Identifiers must be supplied and independently verified. This function cannot verify physical sample provenance.

Usage

```
split_by_experimental_unit(data, unit_id, train_prop = 0.8, seed = NULL)
```

Arguments

data	Data frame containing measurements.
unit_id	Name of verified experimental-unit column.
train_prop	Proportion of unique units for training.
seed	Optional non-negative integer seed. NULL uses and advances the caller's random-number state. An explicit seed gives reproducible results and restores the caller's random-number state.

Value

List containing training data, testing data, and a summary of the split.

---

summarise_dielectric_curves

Summarise dielectric frequency-response curves

Description

Calculates descriptive curve features using the trapezoidal rule over log10(frequency). Curves are defined by material and ageing time. These summaries do not establish independent replication.

Usage

```
summarise_dielectric_curves(data, outcome = "permittivity")
```

Arguments

data	Dielectric measurement data frame.
outcome	Name of a numeric response column.

Value

A data frame containing curve-level summaries.

`summarise_dielectric_variability` *Summarise dielectric measurements without assuming independence*

Description

Calculates descriptive statistics within experimental conditions. Standard errors and confidence intervals are deliberately not calculated because physical sample independence is not established.

Usage

```
summarise_dielectric_variability(
  data,
  outcome = "permittivity",
  group_vars = c("fuel", "water", "concentration_pct", "age_hours")
)
```

Arguments

`data`	A dielectric measurement data frame.
`outcome`	Name of a numeric outcome column.
`group_vars`	Names of grouping columns.

Value

A data frame of descriptive summaries.

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