Package 'PolyMigR'

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Type Package

Title Analysis of Polyphenol Migration from Packaging Films

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Maintainer Tanuj Misra <tanujmisra102@gmail.com>

Description The gradual release of active substances from packaging can enhance food preservation by maintaining high concentrations of polyphenols and antioxidants for a period of 72 hrs. To assess the effectiveness of packaging materials that serve as carriers for antioxidants, it is crucial to model the diffusivity of the active agents. Understanding this diffusivity helps evaluate the packaging's capacity to prolong the shelf life of food items. The process of migration, which encompasses diffusion, dissolution, and reaching equilibrium, facilitates the transfer of low molecular weight compounds from the packaging into food simulants. The rate at which these active compounds are released from the packaging is typically analysed using food simulants under conditions outlined in European food packaging regulations (Ramos et al., 2014).

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Author Anamika Nayak [aut, ctb, cph],
Debjani Dutta [aut, ctb, cph],
Ajaya Rout [aut, ctb, cph],
Tanuj Misra [aut, cre, ctb, cph],
Satya Narayan Parida [aut, ctb, cph]

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Contents

`first_order` *First order empirical model*

Description

The first order empirical model signifies an exponential release profile consistent with Fickian mechanisms rather than a linear one.

Principle:

It is based on the principle that the release rate is directly proportional to the concentration of polyphenol remaining within the film matrix. The migration occurs rapidly at the beginning—when the concentration gradient between the film and the surrounding medium is high—and gradually decreases over time as the active compound becomes depleted (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
first_order(M0, K1, t)
```

Arguments

`M0`	Initial amount of drug released at t=0
`K1`	First-order release rate constant)
`t`	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

Malekjani, N., Karimi, R., Assadpour, E., & Jafari, S. M. (2024). Control of release in active packaging/coating for food products; approaches, mechanisms, profiles, and modeling. Critical reviews in food science and nutrition, 64(29), 10789-10811.

Examples

```
first_order (0.80, 0.025, 24)
```

`higuchi` *Higuchi model*

Description

Higuchi model describes release based on the principle of diffusion-controlled transport from a homogeneous matrix system.

Principle:

This Higuchi model indicates that migration is predominantly governed by Fickian diffusion through the polymer matrix, with the release rate decreasing over time due to the progressive reduction in the concentration gradient and increased diffusion path length (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
higuchi (kH, t)
```

Arguments

`kH`	Higuchi release constant
`t`	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

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Examples

```
higuchi (0.22, 25)
```

`korsmeyer_peppas` *Korsmeyer Peppas model*

Description

The Korsmeyer–Peppas model describes the dominant release mechanism in systems where the exact transport process is complex or not purely diffusion-controlled.

Principle:

Korsmeyer–Peppas model is based on the principle of a power-law relationship between the fraction of active compound released over time. The model introduces a release exponent that characterizes the underlying transport mechanism within the polymer matrix. This exponent indicates whether migration follows Fickian diffusion, anomalous (non-Fickian) transport involving coupled diffusion and polymer relaxation, or case II transport governed primarily by polymer swelling or chain relaxation (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
korsmeyer_peppas (M_infinite, k, t, n)
```

Arguments

`M_infinite`	maximum migrated amount
`k`	a constant that reflects the release rate and is influenced by the properties of the drug and the polymeric matrix
`n`	an exponent that characterizes the release mechanism
`t`	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

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Examples

```
korsmeyer_peppas(2, 0.18, 24, 0.45)
```

peleg *Peleg model*

Description

Peleg model describes both the early-stage release dynamics and the long-term stabilization phase, making it particularly useful for evaluating overall migration performance and predicting equilibrium release behaviour in active packaging systems.

Principle:

This model is based on the principle of an empirical, time-dependent approach that characterizes release behaviour through two kinetic constants representing the initial release rate and the system's approach to equilibrium. The model assumes that the release process is rapid at the initial stage and gradually decreases over time as the system approaches a maximum release capacity (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
peleg (M_infinite, k1, k2, t)
```

Arguments

M_infinite	maximum migrated amount
k1	This constant is associated with first-order kinetics, reflecting the initial release rate
k2	This constant is associated with second-order kinetics. It typically represents the influence of slower processes such as diffusion, polymer swelling, or matrix degradation that affect drug release over time
t	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

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Examples

```
peleg (2, 0.02, 0.015, 24)
```

second_order *Second order empirical model*

Description

A second-order model suggests that release is governed by concentration-dependent interaction dynamics within the polymer network, providing mechanistic insight into matrix reactivity and controlled migration behaviour.

Principle:

The principle of this kinetic behaviour is concentration-dependent and may involve bimolecular interactions, such as polyphenol–polymer binding, association–dissociation equilibria, or other matrix-controlled reactive processes (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
second_order (M_infinite, K, t)
```

Arguments

M_infinite	Total amount of drug that can be released, or the maximum drug capacity of the system
K	Release rate constant, which reflects how quickly the drug is being released from the delivery system
t	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

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Examples

```
second_order(0.767, 0.0164, 72)
```

`weibull` *Weibull model*

Description

Weibull model is significant for describing non-linear and heterogeneous migration behaviour in active packaging systems.

Principle:

Principle of this model lies that polyphenol migration is governed by heterogeneous and possibly multi-mechanistic processes within the polymer matrix, offering a comprehensive description of release kinetics in active packaging systems. It provides a flexible empirical approach capable of describing complex and non-ideal release behaviour that do not strictly follow zero-order, first-order, or Higuchi kinetics (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
weibull (M_infinite, a, b, t)
```

Arguments

`M_infinite`	maximum migrated amount
`a`	constant that reflects the rate of the release process
`b`	an exponent that characterizes the nature of the release mechanism
`t`	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

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Examples

```
weibull (2, 0.015, 0.75, 24)
```

`zero_order` *Zero order empirical model*

Description

The zero-order empirical model signifies that polyphenol migration from the active packaging film occurs at a constant, concentration-independent rate over time.

Principle:

the zero-order model release governed by a constant rate (k0), independent of the remaining concentration of the active compound in the matrix resulting in a linear increase in the cumulative amount of migrated polyphenol with time. It indicates a predictable, sustained, and uniform delivery of polyphenol from the packaging film (Ramos et al., 2014; Malekjani et al., 2024).

Usage

```
zero_order(M0, K0, t)
```

Arguments

`M0`	Initial amount of drug released at t=0
`K0`	Zero-order release rate constant (the constant rate at which the drug is released, typically expressed in units like mg/hour)
`t`	time

Value

Amount of drug released at time t Gallic Acid Equivalents per gram (GAE/gm)

References

Ramos, M., Beltrán, A., Peltzer, M., Valente, A. J., & del Carmen Garrigós, M. (2014). Release and antioxidant activity of carvacrol and thymol from polypropylene active packaging films. LWT-Food Science and Technology, 58(2), 470-477.

Malekjani, N., Karimi, R., Assadpour, E., & Jafari, S. M. (2024). Control of release in active packaging/coating for food products; approaches, mechanisms, profiles, and modeling. Critical reviews in food science and nutrition, 64(29), 10789-10811.

Examples

```
zero_order(0.767, 0.0164, 72)
```

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