Package ‘PUPMSI’

October 12, 2022

Type Package
Title Moisture Sorption Isotherm Modeling Program
Version 0.1.0
Description Contains sixteen moisture sorption isotherm models, which evaluate the fitness of adsorption and desorption curves for further understanding of the relationship between moisture content and water activity. Fitness evaluation is conducted through parameter estimation and error analysis. Moreover, graphical representation, hysteresis area estimation, and isotherm classification through the equation of Blahovec & Yanniotis (2009) <doi:10.1016/j.jfoodeng.2008.08.007> which is based on the classification system introduced by Brunauer et. al. (1940) <doi:10.1021/ja01864a025> are also included for the visualization of models and hysteresis.
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Brunauer-Emmett-Teller (BET) Moisture Sorption Isotherm

Description

Brunauer-Emmett-Teller (BET) is a two-parameter isotherm model used for the optimum moisture content determination for drying and storage stability of foods, and in the food’s surface area estimation.

Usage

BETMSI(WaterAct, AdsorpM, DesorpM)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>WaterAct</td>
<td>the numerical value of Water Activity, which ranges from 0 to 1.</td>
</tr>
<tr>
<td>AdsorpM</td>
<td>the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.</td>
</tr>
<tr>
<td>DesorpM</td>
<td>the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.</td>
</tr>
</tbody>
</table>

Value

the nonlinear regression, parameters, and graphical visualization for the Brunauer-Emmett-Teller (BET) Moisture Sorption Isotherm model.

Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacortе
Chester C. Deocaris
BradleyMSI

References

Examples

```r
WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
BETMSI(WaterAct, AdsorpM, DesorpM)
```

Description
Bradley model is a two-parameter isotherm model that measures polar nature of sorptive surfaces.

Usage

```
BradleyMSI(WaterAct, AdsorpM, DesorpM)
```

Arguments

- `WaterAct`: the numerical value of Water Activity, which ranges from 0 to 1.
- `AdsorpM`: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- `DesorpM`: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for the Bradley Moisture Sorption Isotherm model.

Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris
References


Examples

```r
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
BradleyMSI(WaterAct, AdsorpM, DesorpM)
```

---

**CaurieMSI**

**Caurie Moisture Sorption Isotherm**

Description

Caurie model is a two-parameter isotherm created for calculation of water sorption data of dehydrated foods over a wide range of water activity.

Usage

```r
CaurieMSI(WaterAct, AdsorpM, DesorpM)
```

Arguments

- **WaterAct**: the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM**: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM**: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value

the nonlinear regression, parameters, and graphical visualization for the Caurie Moisture Sorption Isotherm model.

Author(s)

- Benz L. Rivera
- John Carlo F. Panganiban
- Kim M. Villacorte
- Chester C. Deocaris
References

Examples
WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
CaurieMSI(WaterAct, AdsorpM, DesorpM)

GABMSI

Guggenheim-Anderson-de Boer(GAB) Moisture Sorption Isotherm

Description
GAB model is a multimolecular, localized and homogeneous adsorption model, is one of the most versatile models considering multilayer adsorption at high water activity values.

Usage
GABMSI(WaterAct, AdsorpM, DesorpM)

Arguments
WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for the Guggenheim-Anderson-de Boer(GAB) Moisture Sorption Isotherm model.

Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris
References


Examples

```r
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
GABMSI(WaterAct, AdsorpM, DesorpM)
```

HailHorroMSI

Hailwood-Horrobin (HH) Moisture Sorption Isotherm

Description

Hailwood-Horrobin (HH) model is an example of multilayer surface sorption model, is suitable for analysis of experimental wood moisture sorption (WMS) isotherms.

Usage

```r
HailHorroMSI(WaterAct, AdsorpM, DesorpM)
```

Arguments

- **WaterAct**: the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM**: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM**: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value

The nonlinear regression, parameters, and graphical visualization for the Hailwood-Horrobin (HH) Moisture Sorption Isotherm model.
Halsey MSI

Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References


Examples

WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
HailHorroMSI(WaterAct, AdsorpM, DesorpM)

Halsey MSI

Halsey Moisture Sorption Isotherm

Description

Halsey Isotherm is a 2-parameter model which expresses condensation of multilayers at proportionally large distances from the surface considering the assumption that a molecule’s potential energy is inversely proportional to the nth power of its distance from the surface.

Usage

HalseyMSI(WaterAct, AdsorpM, DesorpM)

Arguments

WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value

the nonlinear regression, parameters, and graphical visualization for the Halsey Moisture Sorption Isotherm model.
Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References

Examples
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
HalseyMSI(WaterAct, AdsorpM, DesorpM)

HendersonMSI

Henderson Moisture Sorption Isotherm

Description
Henderson Isotherm is an empirical two-parameter equation for moisture adsorption of food products, useful in predicting moisture content for different water activity levels.

Usage
HendersonMSI(WaterAct, AdsorpM, DesorpM)

Arguments
WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for the Henderson Moisture Sorption Isotherm model.
**HysteresisMSI**

**Author(s)**
Benz L. Rivera  
John Carlo F. Panganiban  
Kim M. Villacorte  
Chester C. Deocaris

**References**

**Examples**
```r
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)  
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)  
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)  
HendersonMSI(WaterAct, AdsorpM, DesorpM)
```

**HysteresisMSI**  
_Hysteresis Area, Brunauer Classification System_

**Description**
Hysteresis area evaluation via trapezoidal approximation.

**Usage**
```r
HysteresisMSI(WaterAct, AdsorpM, DesorpM)
```

**Arguments**
- **WaterAct** the numerical value of Water Activity, which ranges from 0 to 1.  
- **AdsorpM** the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.  
- **DesorpM** the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

**Value**
the measurement of hysteresis, classification of isotherms, and graphical visualization for the observed values of moisture sorption isotherms.
Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References

Examples

WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
HysteresisMSI(WaterAct, AdsorpM, DesorpM)

IgleChiMSI

Iglesias-Chirife Moisture Sorption Isotherm

Description
Iglesias-Chirife Isotherm is an an empirical equation for describing water sorption behavior of various fruits and other sugar-rich foods.

Usage
IgleChiMSI(WaterAct, AdsorpM, DesorpM)

Arguments
WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for the Iglesias-Chirife Moisture Sorption Isotherm model.
KuhnMSI

Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References


Examples

WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
IgleChiMSI(WaterAct, AdsorpM, DesorpM)

---

KuhnMSI

Kuhn Moisture Sorption Isotherm

Description

Kuhn Isotherm is a two-parameter model which contains many defining characteristics wherein each surface site has a different adsorption potential, as well as cluster formations on each site due to increase in partial pressure.

Usage

KuhnMSI(WaterAct, AdsorpM, DesorpM)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>WaterAct</td>
<td>the numerical value of Water Activity, which ranges from 0 to 1.</td>
</tr>
<tr>
<td>AdsorpM</td>
<td>the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.</td>
</tr>
<tr>
<td>DesorpM</td>
<td>the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.</td>
</tr>
</tbody>
</table>

Value

the nonlinear regression, parameters, and graphical visualization for the Kuhn Moisture Sorption Isotherm model.
Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References


Examples

```r
WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0627, 0.0794, 0.0851, 0.1158, 0.1298, 0.1500, 0.1938)
KuhnMSI(WaterAct, AdsorpM, DesorpM)
```

LangmuirMSI  

Description

Langmuir Isotherm is a two-parameter model applicable for unimolecular layers with similar sorption sites. Langmuir’s isotherm is the most crucial equation among the theoretical models, whose basis are the forces acting between the product surface and the condensed water from the vapor as a monomolecular layer.

Usage

```r
LangmuirMSI(WaterAct, AdsorpM, DesorpM)
```

Arguments

- **WaterAct**: the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM**: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM**: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value

the nonlinear regression, parameters, and graphical visualization for the Langmuir Moisture Sorption Isotherm model.
Lewicki2MSI

Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References

tae. In Vitae (Vol. 18, Issue 3). Facultad De Qui??mica Farmace??utica, Universidad de Antioquia.

Saroyda, J. V., Cruz, et al. (2020) <doi:10.1016/S0001-8686(00)00082> Package "PUPAIM" Type
Package Title A Collection of Physical and Chemical Adsorption Isotherm Models Version 0.2.0.
<doi:10.1016/S0001-8686(00)00082>

Examples

WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
LangmuirMSI(WaterAct, AdsorpM, DesorpM)

Lewicki2MSI

Lewicki-2-Parameter Moisture Sorption Isotherm

Description

Lewicki-2-Parameter MSI is a two-parameter sorption model that was developed based on Raoult’s
law, which assumes that water is present either as free water or as water of hydration.

Usage

Lewicki2MSI(WaterAct, AdsorpM, DesorpM)

Arguments

WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which
ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which
ranges from 0 to 1.

Value

the nonlinear regression, parameters, and graphical visualization for Lewicki-2-Parameter model.
Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References

Examples
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.5342, 0.6385, 0.7384, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
Lewicki2MSI(WaterAct, AdsorpM, DesorpM)

Lewicki3MSI

Lewicki-3-Parameter Moisture Sorption Isotherm

Description
The three-parameter Lewicki model is most suitable for describing the sorption characteristics of raw potato, potato starch, starch-sugar and starch-salt gels within specific temperature and water activity ranges.

Usage
Lewicki3MSI(WaterAct, AdsorpM, DesorpM)

Arguments
WaterAct the numerical value of Water Activity, which ranges from 0 to 1.
AdsorpM the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
DesorpM the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for Lewicki-3-Parameter model.
**ModChenMSI**

**Author(s)**

Benz L. Rivera  
John Carlo F. Panganiban  
Kim M. Villacorte  
Chester C. Deocaris

**References**


**Examples**

```r
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)  
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)  
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)  
Lewicki3MSI(WaterAct, AdsorpM, DesorpM)
```

---

**ModChenMSI**

*Modified Chen Moisture Sorption Isotherm*

**Description**

Modified Chen is 2-parameter model related to the drying principle. It is restricted to situations where diffusion is the primary mode of mass transport and is focused on the steady state of the drying equation.

**Usage**

```r
ModChenMSI(WaterAct, AdsorpM, DesorpM)
```

**Arguments**

- **WaterAct**  
  the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM**  
  the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM**  
  the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

**Value**

the nonlinear regression, parameters, and graphical visualization for the Modified Chen Moisture Sorption Isotherm model.
Author(s)
Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References

Examples
```r
WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
ModChenMSI(WaterAct, AdsorpM, DesorpM)
```

Description
An empirical model developed through a series of mathematical equations that consists in a series expansion for sigmoidal curves.

Usage
```r
OswinMSI(WaterAct, AdsorpM, DesorpM)
```

Arguments
- **WaterAct**: the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM**: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM**: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

Value
the nonlinear regression, parameters, and graphical visualization for the Oswin Moisture Sorption Isotherm model.
Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocarيس

References


Examples

```
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
OswinMSI(WaterAct, AdsorpM, DesorpM)
```

---

**PelegMSI**  
*Peleg Moisture Sorption Isotherm*

**Description**

Peleg model is an empirical 4-parameter isotherm which describes sigmoidal and non-sigmoidal behavior of isotherm plots.

**Usage**

```
PelegMSI(WaterAct, AdsorpM, DesorpM)
```

**Arguments**

- `WaterAct`: the numerical value of Water Activity, which ranges from 0 to 1.
- `AdsorpM`: the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- `DesorpM`: the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

**Value**

the nonlinear regression, parameters, and graphical visualization for the Peleg Moisture Sorption Isotherm model.
SmithMSI

Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References


Examples

```r
WaterAct <- c(0.1145,0.2274,0.3265,0.4291,0.6342,0.7385,0.8274,0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298,0.1500, 0.1938)
PelegMSI(WaterAct, AdsorpM, DesorpM)
```

**Description**

Smith MSI is an empirical isotherm model for curve assessment of water sorption of polymers with high molar mass.

**Usage**

```r
SmithMSI(WaterAct, AdsorpM, DesorpM)
```

**Arguments**

- **WaterAct** the numerical value of Water Activity, which ranges from 0 to 1.
- **AdsorpM** the numerical value of the Moisture content of the Adsorption curve, which ranges from 0 to 1.
- **DesorpM** the numerical value of the Moisture content of the Desorption curve, which ranges from 0 to 1.

**Value**

the nonlinear regression, parameters, and graphical visualization for the Smith Moisture Sorption Isotherm model.
Author(s)

Benz L. Rivera
John Carlo F. Panganiban
Kim M. Villacorte
Chester C. Deocaris

References


Examples

```r
WaterAct <- c(0.1145, 0.2274, 0.3265, 0.4291, 0.6342, 0.7385, 0.8274, 0.9573)
AdsorpM <- c(0.0234, 0.0366, 0.0496, 0.0648, 0.0887, 0.1096, 0.1343, 0.1938)
DesorpM <- c(0.0459, 0.0637, 0.0794, 0.0884, 0.1158, 0.1298, 0.1500, 0.1938)
SmithMSI(WaterAct, AdsorpM, DesorpM)
```
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