Package 'geofluidprop'

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Version 1.2

Type Package

Title R wrapper for the geofluidprop library

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Description An R wrapper for the geofluidprop library for computing physical properties of geological fluids.

License GPL (>= 3)

URL https://github.com/aist-rerc-geothermal/geofluidprop-R

Depends R (>= 3.0.0)

Imports dplyr,
ggplot2,
rlang

RoxygenNote 7.2.2

Encoding UTF-8

Suggests testthat,
knitr,
rmarkdown,

VignetteBuilder knitr

R topics documented:

driesner07_H2O_NaCl_estimate_density_from_M0

Estimate density from concentration

Description

Estimate density from concentration

Usage

```
driesner07_H2O_NaCl_estimate_density_from_M0(M0)
```

Arguments

M0	Molar concentration at room temperature [mol/L]

Value

density [kg/m3]

driesner07_H2O_NaCl_get_phase_relation_on_Tp_space

get information about H2O-NaCl phase relation at the given NaCl mass fraction, based on Driesner & Heinrich (2007)

Description

get information about H2O-NaCl phase relation at the given NaCl mass fraction, based on Driesner & Heinrich (2007)

Usage

```
driesner07_H2O_NaCl_get_phase_relation_on_Tp_space(massfrac_NaCl, TC_max = 800)
```

Arguments

massfrac_NaCl	NaCl mass fraction (bulk) [kg/kg]
TC_max	Maximum temperature to be calculated [K]

Value

a list object including all the phase relation information

driesner07_H2O_NaCl_get_properties_TpX

Get H2O-NaCl fluid properties at the given temperature, pressure, and NaCl mass fraction

Description

Get H2O-NaCl fluid properties at the given temperature, pressure, and NaCl mass fraction

Usage

```
driesner07_H2O_NaCl_get_properties_TpX(TK, p, X, print = FALSE)
```

Arguments

TK	Temeprature [K]
p	Pressure [Pa]
X	Bulk NaCl mass fraction [kg/kg]
print	TRUE for printing the calculated properties

Value

a nested list object including the fluid properties

driesner07_H2O_NaCl_get_Tp_curve_on_F_VL_boundary

get an array of T and p values along a phase boundary between F and VL regions

Description

get an array of T and p values along a phase boundary between F and VL regions

Usage

```
driesner07_H2O_NaCl_get_Tp_curve_on_F_VL_boundary(massfrac_NaCl, TCmax)
```

Arguments

massfrac_NaCl	NaCl mass fraction (bulk) [kg/kg]
TCmax	Maximum temperature to be calculated [K]

Value

dataframe object including calculated TK and p values

driesner07_H2O_NaCl_get_Tp_curve_on_VL_VH_boundary

get an array of T and p values along a phase boundary between VL and VH regions

Description

get an array of T and p values along a phase boundary between VL and VH regions

Usage

```
driesner07_H2O_NaCl_get_Tp_curve_on_VL_VH_boundary(TCmax, n = 50)
```

Arguments

TCmax	Maximum temperature to be calculated [K]
n	the number of sampling temperatures

Value

dataframe object including calculated TK and p values

driesner07_H2O_NaCl_LH_xl_Tp

Saturated liquid composition at L+H coexisting, Function of Temperature and Pressure

Description

The function returns the saturated liquid composition at L+Halite coexisting surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_LH_xl_Tp(TK, p)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]

Value

Mole fraction [-]

`driesner07_H2O_NaCl_pc_T`

Critical pressuer of H2O-NaCl fluid as a function of temperature

---

Description

Returns critical pressure of H2O-NaCl fluid at the given temperature

Usage

```
driesner07_H2O_NaCl_pc_T(TK)
```

Arguments

`TK`	Temperature [K]

Value

Critical pressure [Pa]

`driesner07_H2O_NaCl_pc_T2`

Critical pressuer of H2O-NaCl fluid as a function of temperature using saturation pressure of water below critical temperature

---

Description

Returns critical pressure of H2O-NaCl fluid at the given temperature

Usage

```
driesner07_H2O_NaCl_pc_T2(TK)
```

Arguments

`TK`	Temperature [K]

Value

Critical pressure [Pa]

driesner07_H2O_NaCl_phase_Tpx

Phase id of H2O-NaCl fluid as a function of temperature, pressure, and NaCl composition

Description

Returns phase id of H2O-NaCl fluid at the given temperature, pressure, and bulk salinity

Usage

```
driesner07_H2O_NaCl_phase_Tpx(TK, p, x)
```

Arguments

TK	Temeprature [K]
p	Pressure [Pa]
x	Bulk composition (mole fraction) of NaCl [mol/mol]

Value

phase id

driesner07_H2O_NaCl_plot_phase_relation_on_Tp_space

plot H2O-NaCl phase diagram on T-p space

Description

plot H2O-NaCl phase diagram on T-p space

Usage

```
driesner07_H2O_NaCl_plot_phase_relation_on_Tp_space(dat, TC_range_max = 800)
```

Arguments

dat	H2O-NaCl phase relation information
TC_range_max	Maximum temperature to be plotted [K]

`driesner07_H2O_NaCl_rho_pTx`

Salinewater density, Function of Temperature, Pressure, and composition

---

Description

The function returns the saline water density for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_rho_pTx(p, TK, x)
```

Arguments

`p`	Pressure [Pa]
`TK`	Temperature [K]
`x`	Mole fraction [-]

Value

Density [kg/m3]

`driesner07_H2O_NaCl_rho_singlephase_pTx`

Salinewater density, Function of Temperature, Pressure, and composition

---

Description

The function returns the saline water density for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_rho_singlephase_pTx(p, TK, x)
```

Arguments

`p`	Pressure [Pa]
`TK`	Temperature [K]
`x`	Mole fraction [-]

Value

Density [kg/m3]

driesner07_H2O_NaCl_singlephase_h_Tpx

Salinewater Specific Enthalphy, Function of Temperature, Pressure, and composition

Description

The function returns the saline water specific enthalpy for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_singlephase_h_Tpx(TK, p, x)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]
x	Mole fraction [-]

Value

Specific Enthalpy [J/kg]

driesner07_H2O_NaCl_singlephase_p_rhoTx

calculate pressure from salinewater density and salinity

Description

calculate pressure from salinewater density and salinity

Usage

```
driesner07_H2O_NaCl_singlephase_p_rhoTx(rho, TK, x, pVL, pmax = 5e+08)
```

Arguments

rho	Density [kg/m^3]
TK	Temperature [K]
x	Mole fraction [-]
pVL	V-L pressure used as lower bound [Pa]
pmax	upper bound of pressure [Pa]

Value

pressure [Pa]

`driesner07_H2O_NaCl_Tc_x`

Critical temperature of H2O-NaCl fluid as a function of NaCl composition

---

Description

Returns critical temperature of H2O-NaCl fluid at the given composition

Usage

```
driesner07_H2O_NaCl_Tc_x(x)
```

Arguments

`x`	Composition (mole fraction) of NaCl [mol/mol]

Value

Temperature [K]

`driesner07_H2O_NaCl_VH_vol_frac_h`

Halite volume fraction in V+H phase

Description

The function returns the solid volume fraction in V+H phase for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_VH_vol_frac_h(TK, p, x)
```

Arguments

`TK`	Temperature [K]
`p`	Pressure [Pa]
`x`	NaCl composition [mol/mol]

Value

Volume fraction [m3/m3]

driesner07_H2O_NaCl_VH_xv_Tp

Saturated vapor composition at V+H coexisting, Function of Temperature and Pressure

Description

The function returns the saturated vapor composition at V+Halite coexisting surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_VH_xv_Tp(TK, p)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]

Value

Mole fraction [-]

driesner07_H2O_NaCl_VLH_p_T

Saturation pressure at V+L+H surface, Function of Temperature

Description

The function returns the saturation pressure at V+L+Halite coexisting surface for given temperature.

Usage

```
driesner07_H2O_NaCl_VLH_p_T(TK)
```

Arguments

TK	Temperature [K]

Value

Pressure [Pa]

driesner07_H2O_NaCl_VLH_T_xv

get temperature of VLH curve at the given vapor x

Description

get temperature of VLH curve at the given vapor x

Usage

```
driesner07_H2O_NaCl_VLH_T_xv(xv)
```

Arguments

xv	NaCl composition (mole fraction) of vapor [mol/mol]

Value

Temperature [K]

driesner07_H2O_NaCl_VLH_xl_T

Saturated liquid composition at V+L+H surface, Function of Temperature

Description

The function returns the saturated liquid composition at V+L+Halite coexisting surface for given temperature.

Usage

```
driesner07_H2O_NaCl_VLH_xl_T(TK)
```

Arguments

TK	Temperature [K]

Value

Mole fraction [-]

driesner07_H2O_NaCl_VLH_xv_T

Saturated vapor composition at V+L+H surface, Function of Temperature

Description

The function returns the saturated vapor composition at V+L+Halite coexisting surface for given temperature.

Usage

```
driesner07_H2O_NaCl_VLH_xv_T(TK)
```

Arguments

TK	Temperature [K]

Value

Mole fraction [-]

driesner07_H2O_NaCl_VL_mass_frac_l

Liquid mass fraction in V+L phase

Description

The function returns the liquid mass fraction in V+L phase for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_VL_mass_frac_l(TK, p, x)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]
x	NaCl composition [mol/mol]

Value

Mass fraction [kg/kg]

`driesner07_H2O_NaCl_VL_mass_frac_v`
Vapor mass fraction in V+L phase

Description

The function returns the vapor mass fraction in V+L phase for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_VL_mass_frac_v(TK, p, x)
```

Arguments

`TK`	Temperature [K]
`p`	Pressure [Pa]
`x`	NaCl composition [mol/mol]

Value

Mass fraction [kg/kg]

`driesner07_H2O_NaCl_VL_pl_Tx`
get liquid phase pressure in V+L region at the given T and x

Description

get liquid phase pressure in V+L region at the given T and x

Usage

```
driesner07_H2O_NaCl_VL_pl_Tx(TK, x)
```

Arguments

`TK`	Temperature [K]
`x`	Bulk composition (mole fraction) of NaCl [mol/mol]

Value

a list of liquid pressures [Pa]

driesner07_H2O_NaCl_VL_pv_Tx

get vapor phase pressure(s) in V+L region at the given T and x

Description

get vapor phase pressure(s) in V+L region at the given T and x

Usage

```
driesner07_H2O_NaCl_VL_pv_Tx(TK, x)
```

Arguments

TK	Temperature [K]
x	Bulk composition (mole fraction) of NaCl [mol/mol]

Value

a list of vapor pressures [Pa]

driesner07_H2O_NaCl_VL_rhol_Tp

Saturated liquid density at V+L surface, Function of Temperature and Pressure

Description

The function returns the saturated liquid density at V+L surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_VL_rhol_Tp(TK, p)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]

Value

Density [kg/m3]

`driesner07_H2O_NaCl_VL_rhov_Tp`

Saturated vapor density at V+L surface, Function of Temperature and Pressure

---

Description

The function returns the saturated vapor density at V+L surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_VL_rhov_Tp(TK, p)
```

Arguments

`TK`	Temperature [K]
`p`	Pressure [Pa]

Value

Density [kg/m3]

`driesner07_H2O_NaCl_VL_vol_frac_l`

Liquid volume fraction in V+L phase

Description

The function returns the liquid volume fraction in V+L phase for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_VL_vol_frac_l(TK, p, x)
```

Arguments

`TK`	Temperature [K]
`p`	Pressure [Pa]
`x`	NaCl composition [mol/mol]

Value

Volume fraction [m3/m3]

driesner07_H2O_NaCl_VL_vol_frac_v

Vapor volume fraction in V+L phase

Description

The function returns the vapor volume fraction in V+L phase for given temperature, pressure, and composition.

Usage

```
driesner07_H2O_NaCl_VL_vol_frac_v(TK, p, x)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]
x	NaCl composition [mol/mol]

Value

Volume fraction [m3/m3]

driesner07_H2O_NaCl_VL_xl_Tp

Saturated liquid composition at V+L surface, Function of Temperature and Pressure

Description

The function returns the saturated liquid composition at V+L surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_VL_xl_Tp(TK, p)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]

Value

Mole fraction [-]

driesner07_H2O_NaCl_VL_xv_Tp

Saturated vapor composition at V+L surface, Function of Temperature and Pressure

Description

The function returns the saturated vapor composition at V+L surface for given temperature and pressure.

Usage

```
driesner07_H2O_NaCl_VL_xv_Tp(TK, p)
```

Arguments

TK	Temperature [K]
p	Pressure [Pa]

Value

Mole fraction [-]

driesner07_H2O_NaCl_write_phase_relation_on_Tp_space

save H2O-NaCl phase relations on T-p space to a text file

Description

save H2O-NaCl phase relations on T-p space to a text file

Usage

```
driesner07_H2O_NaCl_write_phase_relation_on_Tp_space(dat, filename)
```

Arguments

dat	H2O-NaCl phase relation information
filename	Output file name

`driesner07_H2O_NaCl_xc_T` *Critical NaCl composition of H2O-NaCl fluid as a function of temperature*

Description

Returns critical composition of H2O-NaCl fluid at the given temperature

Usage

```
driesner07_H2O_NaCl_xc_T(TK)
```

Arguments

`TK`	Temperature [K]

Value

Critical composition (mole fraction) of NaCl [mol/mol]

`geofluidprop` *geofluidprop*

Description

A library for computing physical properties of geological fluids

`H2ONaCl_b_to_M` *Convert H2O-NaCl concentration unit from molality to mole fraction*

Description

Convert concentration unit of saline water

Usage

```
H2ONaCl_b_to_M(m, rho = 998.2)
```

Arguments

`m`	molality [mol/kg-H2O]
`rho`	density [kg/m3]

Value

Molar concentration [mol/L]

H2ONaCl_b_to_massfrac *Convert H2O-NaCl concentration unit from molality to mass fraction*

Description

Convert H2O-NaCl concentration unit from molality to mass fraction

Usage

```
H2ONaCl_b_to_massfrac(b)
```

Arguments

b	molality [mol/kg-H2O]

Value

mass fraction of NaCl [kg/kg]

H2ONaCl_b_to_x *Convert H2O-NaCl concentration unit from molality to mole fraction*

Description

Convert concentration unit of saline water

Usage

```
H2ONaCl_b_to_x(molality)
```

Arguments

molality	molality [mol/kg-H2O]

Value

Mole fraction [-]

H2ONaCl_ec_SakumaIchiki2016_highP

H2O-NaCl fluid electrical conductivity model in Sakuma and Ichiki (2016) for high pressures

Description

The model is valid for 0.2-2 GPa, 673-2000K, 0.6-9.6wt%.

Usage

```
H2ONaCl_ec_SakumaIchiki2016_highP(p, T, c)
```

Arguments

p	Pressure [MPa]
T	Temperature [K]
c	Salinity [wt%]

Value

Electrical conductivity [ohm^-1 m^-1]

References

Sakuma, H., Ichiki, M. (2016) Electrical conductivity of NaCl-H2O fluid in the crust. JGR Solid Earth.

H2ONaCl_ec_SakumaIchiki2016_lowP

H2O-NaCl fluid electrical conductivity model in Sakuma and Ichiki (2016) for low pressures

Description

The model is valid for <0.2 GPa, <600K, 0.6-9.6wt% NaCl

Usage

```
H2ONaCl_ec_SakumaIchiki2016_lowP(p, TK, c)
```

Arguments

p	Pressure [MPa]
TK	Temperature [K]
c	Salinity [wt%]

Value

Electrical conductivity [ohm^-1 m^-1]

References

Sakuma, H., Ichiki, M. (2016) Electrical conductivity of NaCl-H2O fluid in the crust. JGR Solid Earth.

`H2ONaCl_ec_SenGoode1992`

H2O-NaCl fluid electrical conductivity model by Sen & Goode (1992)

Description

The model is valid for 20-200 C.

Usage

```
H2ONaCl_ec_SenGoode1992(m, TC)
```

Arguments

`m`	NaCl molality [mol/kg]
`TC`	Temperature [deg C]

Value

Electrical conductivity [S/m]

References

Sen, P.N., Goode, P.A. (1992) Influence of temperature on electrical conductivity of shaly sands, Geophysics 57 (1), 89–96.

Sen, P.N., Goode, P.A. (1992) Errata, to “influence of temperature on electrical conduc- tivity of shaly sands”, Geophysics 57 (12), 1658.

`H2ONaCl_ec_SinmyoKeppler2017` *H2O-NaCl fluid electrical conductivity model by Sinmyo and Keppler (2017)*

Description

H2O-NaCl fluid electrical conductivity model by Sinmyo and Keppler (2017)

Usage

```
H2ONaCl_ec_SinmyoKeppler2017(pMPa, TK, c_wtp)
```

Arguments

`pMPa`	Pressure [MPa]
`TK`	Temperature [K]
`c_wtp`	Salinity [wt%]

Value

Electrical conductivity [ohm^-1 m^-1]

References

Sinmyo, R., Keppler, H. (2017) Electrical conductivity of NaCl-bearing aqueous fluids to 600C and 1GPa. Contrib Mineral Petrol 172:4

`H2ONaCl_ec_WatanabeEtAl2021_Tpm` *H2O-NaCl fluid electrical conductivity model in Watanabe et al (2021, FPE)*

Description

H2O-NaCl fluid electrical conductivity model in Watanabe et al (2021, FPE)

Usage

```
H2ONaCl_ec_WatanabeEtAl2021_Tpm(TK, pMPa, m)
```

Arguments

`TK`	Temperature [K]
`pMPa`	Pressure [MPa]
`m`	NaCl molality [mol/kg-H2O]

Value

Electrical conductivity [S/m]

`H2ONaCl_massfrac_to_b` *Convert H2O-NaCl concentration unit from mass fraction to molality*

Description

Convert H2O-NaCl concentration unit from mass fraction to molality

Usage

```
H2ONaCl_massfrac_to_b(X)
```

Arguments

`X`	Mass fraction [kg/kg]

Value

molality [mol/kg-H2O]

`H2ONaCl_massfrac_to_M` *Convert H2O-NaCl concentration unit from mass fraction to molar concentration*

Description

Convert H2O-NaCl concentration unit from mass fraction to molar concentration

Usage

```
H2ONaCl_massfrac_to_M(X, rho = 998.2)
```

Arguments

`X`	Mass fraction [kg/kg]
`rho`	Solution density [kg/m3]

Value

Molar concentraion [mol/L]

H2ONaCl_massfrac_to_x *Convert H2O-NaCl concentration unit from mass fraction to mole fraction*

Description

Convert concentration unit of saline water

Usage

```
H2ONaCl_massfrac_to_x(mass_frac)
```

Arguments

mass_frac	Mass fraction [-]

Value

Mole fraction [-]

H2ONaCl_molar_ec_WatanabeEtAl2021_vism *Molar electrical conductivity model of H2O-NaCl fluids in Watanabe et al (2021, FPE)*

Description

Molar electrical conductivity model of H2O-NaCl fluids in Watanabe et al (2021, FPE)

Usage

```
H2ONaCl_molar_ec_WatanabeEtAl2021_vism(vis, m)
```

Arguments

vis	viscosity [Pa s]
m	NaCl molality [mol/kg-H2O]

Value

Molar conductivity [Sm^2/mol]

`H2ONaCl_M_to_b` *Convert H2O-NaCl concentration unit from molar concentration to mass fraction*

Description

Convert concentration unit of saline water from molar concentration to mass fraction

Usage

```
H2ONaCl_M_to_b(M, rho = 998.2)
```

Arguments

`M`	Molar concentraion [mol/L] = [M]
`rho`	Solution density [kg/m3]

Value

molality [mol/kg-H2O]

`H2ONaCl_M_to_massfrac` *Convert H2O-NaCl concentration unit from molar concentration to mass fraction*

Description

Convert concentration unit of saline water from molar concentration to mass fraction

Usage

```
H2ONaCl_M_to_massfrac(M, rho = 998.2)
```

Arguments

`M`	Molar concentraion [mol/L] = [M]
`rho`	Solution density [kg/m3]

Value

Mass fraction [kg/kg]

H2ONaCl_M_to_x — *Convert H2O-NaCl concentration unit from molar concentration to molar fraction*

Description

Convert H2O-NaCl concentration unit from molar concentration to molar fraction

Usage

```
H2ONaCl_M_to_x(M, rho = 998.2)
```

Arguments

M	Molarity [mol/L]
rho	Solution density [kg/m3]

Value

Mole fraction of NaCl [mol/mol]

H2ONaCl_x_to_massfrac — *Convert H2O-NaCl concentration unit from mole fraction to mass fraction*

Description

Convert concentration unit of saline water

Usage

```
H2ONaCl_x_to_massfrac(mole_frac)
```

Arguments

mole_frac	Mole fraction [-]

Value

Mass fraction [-]

iapws95_rho_pT *Water density using IAPWS-95*

Description

Water density using IAPWS-95

Usage

```
iapws95_rho_pT(pPa, TK)
```

Arguments

pPa	pressure [Pa]
TK	Temperature [K]

Value

water density [kg/m^3]

klyukinetal2017_H2O_NaCl_viscosity_rhoTx *Dynamic Viscosity of Salinewater, Function of Density, Temperature, and Salinity*

Description

Dynamic Viscosity of Salinewater, Function of Density, Temperature, and Salinity

Usage

```
klyukinetal2017_H2O_NaCl_viscosity_rhoTx(rho, TK, x)
```

Arguments

rho	Fluid density [kg/m3]
TK	Temperature [K]
x	Salinity in mole fraction [mol/mol]

Value

Dynamic viscosity [Pa s]

References

Klyukin, Y.I., Lowell R.P., Bodnar, R.J. (2017) A revised empirical model to calculate the dynamic viscosity of H2O-NaCl fluids at elevated temperatures and pressures (<=1000 C, <=500 MPa, 0-100 wt Equilibria 433, 193-205.

`printf` *C-like printf*

Description

C-like printf

Usage

```
printf(...)
```

Arguments

`...`	arguments

`toC` *convert temperature in Kelvin to degree C*

Description

convert temperature in Kelvin to degree C

Usage

```
toC(TK)
```

Arguments

`TK`	temperature in K

Value

temperature in deg C

toK *convert temperature in degree C to Kelvin*

Description

convert temperature in degree C to Kelvin

Usage

```
toK(TC)
```

Arguments

TC	temperature in deg C

Value

temperature in K

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