KCE

ThermoFluidProperties

Property Library for Liquid Secondary Refrigerants Calculated from the IIR Formulation 2010

LibSecRef

Prof. Hans-Joachim Kretzschmar
Dr. Sebastian Herrmann
Dr. Matthias Kunick
Tobias Göpfert
Martin Sünder

Program Functions

Property Functions

The LibSecRef property library uses the formulation for liquid secondary refrigerants by Melinder [1, 2]. The secondary refrigerants presented in this library are water solutions without other additives. The chemical sum formulas of the solute are given in Table 0.1 and the values for the range of validities for mass fraction and temperatures for these solutions are given in Section 0. The property library has been developed by Göpfert [3] in 2012 and revised by Sünder [4] in 2017.

Table 0.1: Chemical sum formula and value of *I_TYPE* for the solutes

Name of solute	**Chemical sum formula**	***I_TYPE***
Ethylene glycol	$C_2H_6O_2$	1
Propylene glycol	$C_3H_8O_2$	2
Ethyl alcohol	C_2H_5OH	3
Methyl alcohol	CH_3OH	4
Glycerol	$C_3H_8O_3$	5
Potassium carbonate	K_2CO_3	6
Calcium chloride	$CaCl_2$	7
Magnesium chloride	$MgCl_2$	8
Sodium chloride	NaCl	9
Potassium acetate	$C_2H_3KO_2$	10
Potassium formate	$CHKO_2$	11
Lithium chloride	LiCl	12
Ammonia	NH_3	13

Within the property library LibSecRef, backwards equations for the calculation of the solution temperature as a function of pressure, mass fraction and specific volume, specific entropy or specific enthalpy are available, too.

The reference state is at mass fraction $\xi = 0$ (pure water), at temperature t = 0°C, and for specific entropy at the pressure p = 101,325 kPa. The reference values for specific enthalpy, specific internal energy, and specific entropy correspond to the IAPWS-IF97 Industrial Formulation for Water [5, 6]. These values are a specific enthalpy of $h = 0.06101\,\mathrm{kJ\,kg^{-1}}$ and a specific entropy of $s = -0.0001477\,\mathrm{kJ\,kg^{-1}\,K^{-1}}$.

The thermodynamic and transport property functions of the LibSecRef property library shown in Table 0.2 are available as functions of the pressure p in bar, the temperature of the solution t in °C and the mass fraction of the solute ξ in $\mathrm{kg\,kg^{-1}}$. In addition, the property library contains a function to calculate the mass fraction ξ as a function of the freezing temperature of the solution t_f in °C and a function to calculate the freezing temperature t_f as a function of the mass fraction ξ. To call a specific solute of the solution, the value *I_TYPE* is used. All functions can be applied in the entire range of validity shown in Table 0.3.

Table 0.2: Functions of the property library LibSecRef

Functional dependence	**Function Name**	**Call from DLL LibSecRef, Result as Parameter**	**Property**	**Unit**
a = f(*I_TYPE*, p, t, ξ)	a_ptxi_SecRef	= A_PTXI_SECREF(I_TYPE,P,T,XI)	Thermal diffusivity	$m^2\ s^{-1}$
α_v = f(*I_TYPE*, p, t, ξ)	alfav_ptxi_SecRef	= ALFAV_PTXI_SECREF(I_TYPE,P,T,XI)	Isobaric cubic expansion coefficient	K^{-1}
c_p = f(*I_TYPE*, p, t, ξ)	cp_ptxi_SecRef	= CP_PTXI_SECREF(I_TYPE,P,T,XI)	Specific isobaric heat capacity	$kJ\ kg^{-1}\ K^{-1}$
η = f(*I_TYPE*, p, t, ξ)	eta_ptxi_SecRef	= ETA_PTXI_SECREF(I_TYPE,P,T,XI)	Dynamic viscosity	Pa s
h = f(*I_TYPE*, p, t, ξ)	h_ptxi_SecRef	= H_PTXI_SECREF(I_TYPE,P,T,XI)	Specific enthalpy	$kJ\ kg^{-1}$
λ = f(*I_TYPE*, p, t, ξ)	lam_ptxi_SecRef	= LAM_PTXI_SECREF(I_TYPE,P,T,XI)	Thermal conductivity	$W\ m^{-1}\ K^{-1}$
v = f(*I_TYPE*, p, t, ξ)	ny_ptxi_SecRef	= NY_PTXI_SECREF(I_TYPE,P,T,XI)	Kinematic viscosity	$m^2\ s^{-1}$
Pr = f(*I_TYPE*, p, t, ξ)	Pr_ptxi_SecRef	= PR_PTXI_SECREF(I_TYPE,P,T,XI)	Prandtl number	-
ρ = f(*I_TYPE*, p, t, ξ)	rho_ptxi_SecRef	= RHO_PTXI_SECREF(I_TYPE,P,T,XI)	Density	$kg\ m^{-3}$
s = f(*I_TYPE*, p, t, ξ)	s_ptxi_SecRef	= S_PTXI_SECREF(I_TYPE,P,T,XI)	Specific entropy	$kJ\ kg^{-1}\ K^{-1}$
t = f(*I_TYPE*, p, h, ξ)	t_phxi_SecRef	= T_PHXI_SECREF(I_TYPE,P,H,XI)	Backward function: Temperature from pressure, specific enthalpy, and mass fraction	°C
t = f(*I_TYPE*, p, s, ξ)	t_psxi_SecRef	= T_PSXI_SECREF(I_TYPE,P,S,XI)	Backward function: Temperature from pressure, specific entropy, and mass fraction	°C
t = f(*I_TYPE*, p, v, ξ)	t_pvxi_SecRef	= T_PVXI_SECREF(I_TYPE,P,V,XI)	Backward function: Temperature from pressure, specific volume, and mass fraction	°C
t_f = f(*I_TYPE*, ξ)	tf_xi_SecRef	= TF_XI_SECREF(I_TYPE,XI)	Freezing temperature	°C
u = f(*I_TYPE*, p, t, ξ)	u_ptxi_SecRef	= U_PTXI_SECREF(I_TYPE,P,T,XI)	Specific internal energy	$kJ\ kg^{-1}$
v = f(*I_TYPE*, p, t, ξ)	v_ptxi_SecRef	= V_PTXI_SECREF(I_TYPE,P,T,XI)	Specific volume	$m^3\ kg^{-1}$
ξ = f(*I_TYPE*, t_f)	xi_tf_SecRef	= XI_TF_SECREF(I_TYPE,TF)	Mass fraction of the solute	$kg\ kg^{-1}$

Range of Validity

The input parameters must always be:

I_TYPE : $1 \le I\_TYPE \le 13$

p : $0 < p \le 100\ \text{bar}$ (for liquid solution)

t : $t \ge t_\text{f}$ and $\begin{cases} t_\text{f,min} \le t \le t_\text{b,max} & \text{for } I\_TYPE = 1,2,5\ldots10,12 \\ t_\text{f,min} \le t \le 100°\text{C} & \text{for } I\_TYPE = 3,4,13 \\ t_\text{f,min} \le t \le t_\text{max,[1,2]} & \text{for } I\_TYPE = 11 \end{cases}$

ξ : $0 \le \xi \le \xi_\text{max}$

The values for the minimum and maximum values are given in Table 0.3.

Note:

If the calculation results in –1000, the values entered represent a state point beyond the range of validity. For further information on each function and its range of validity, see Chapter 3. The same information may be accessed via the online help pages.

The temperature t have to be between the freezing temperature t_f and the maximum temperature t_max, whereas the freezing temperature also represents the minimum temperature of the solution at ξ_max and t_max is in most cases equal to the boiling temperature $t_\text{b,max}$ at ξ_max. The temperature and mass fraction ranges of the functions of LibSecRef are shown in Table 0.3.

This property library contains an extension of the range of validity with respect to maximum (boiling) temperature $t_\text{b,max}$ of the solution in comparison with the maximum temperatures given by Melinder [1, 2], except for potassium formate. The extension can be seen from Table 0.3 when comparing the temperature values of column $t_\text{max,[1,2]}$ given by Melinder and $t_\text{b,max}$ at ξ_max. The temperature values $t_\text{b,max}$ where calculated using polynomials up to the fifth order. The polynomials were fitted to experimental data for mass fraction and boiling temperatures from literature [1, 2]. Sünder [4] described the results in detail. The equation for the boiling temperature $t_{\text{b}i}$ of the i-th water solution reads

$$t_{\text{b}i} = 100°\text{C} + \left(\sum_{j=1}^{5} n_{ij} \cdot \xi_i^j \right) \cdot \text{K}\,, \tag{0.1}$$

where n_{ij} are the coefficients given in

Table 0.4 for each solute except potassium formate, ξ_i is the mass fraction of the solute of the i-th water solution, and $i = I\_TYPE$ with $1 \le i \le 13$ and $i \ne 11$. It is to note, that the uncertainty of the calculated properties increases for temperatures greater than the maximum temperature $t_\text{max,[1,2]}$ given by Melinder.

Table 0.3: Values for the range of validity for mass fraction and temperatures

Name of solute	ξ_{max}	$t_{min} = t_{f,min}$	$t_{max} = t_{b,max}$	$t_{max,[1,2]}$	I_TYPE
	kg kg^{-1}	°C	°C	°C	
Ethylene glycol	0.60	−51.2	110.5	100	1
Propylene glycol	0.60	−50.0	109.1	100	2
Ethyl alcohol	0.60	−44.9	80.6	40	3
Methyl alcohol	0.60	−73.0	74.1	40	4
Glycerol	0.67	−46.5	111.8	40	5
Potassium carbonate	0.40	−37.5	108.0	40	6
Calcium chloride	0.30	−48.0	110.5	40	7
Magnesium chloride	0.215	−33.6	108.1	40	8
Sodium chloride	0.234	−21.1	106.3	40	9
Potassium acetate	0.45	−52.0	112.5	40	10
Potassium formate	0.48	-50.0	-	40	11
Lithium chloride	0.24	-62.9	111.5	40	12
Ammonia	0.30	-84.1	27.5	30	13

Table 0.4: Coefficients n_{ij} used in Eq. (0.1) with $i = I\_TYPE$

	j				
i	1	2	3	4	5
1	7.81415903	−19.9229957	113.363404	−119.782128	51.5110171
2	4.94479449	4.13206053	21.6258504	0	0
3	−120.680009	368.801426	−621.968290	519.215854	−163.191803
4	−103.090685	215.227069	−272.119940	114.700035	30.9228031
5	11.6924190	−56.9602147	250.010758	−396.349972	253.505904
6	12.3813527	−34.3365389	159.024248	−76.0614813	27.9822552
7	22.0989620	−132.647857	1416.18758	−4679.99034	6365.87966
8	24.1369594	−63.4247892	1496.00609	−8440.87786	19713.2539
9	15.9829730	−21.3491122	373.371212	160.146576	−2226.17439
10	16.9026646	9.02824466	62.3843436	−189.871937	280.054850
11*					
12	−14.0198990	859.410555	−6821.50899	27735.1915	−40686.4855
13	−407.074975	1350.83131	−5225.96579	10617.0252	−6936.99691

* No experimental values available