

LiBrSSC (aqueous lithium bromide) Property Routines

The property routines described here are for the aqueous salt mixture LiBr/H₂O. These routines were developed primarily as a part of the Sorption Systems Consortium at the University of Maryland.

The basic routines are provided in an external library named LiBrSSC.dll. The routines available in this library are listed in Table 1. The units of the properties must be as specified.

Table 1. Summary of LiBrSSC Routines

Functions	OutputUnits	
Thermal conductivity	W/m-K	$k = \text{LiBrSSCCond}(T_c, X)$
Dynamic viscosity	cP	$\mu = \text{LiBrSSCVisc}(T_c, X)$
Specific heat	J/g-K	$c_p = \text{LiBrSSCCp}(T_c, X, P)$ or $cp_{\text{sat}} = \text{LiBrSSCCp}(T_c, X)$
Enthalpy	J/g	$h = \text{LiBrSSCh}(T_c, X, P)$ or $h_{\text{sat}} = \text{LiBrSSCh}(T_c, X)$
Chemical potential of water	J/g	$\mu_w = \text{LiBrSSCuw}(T_c, X, P)$
Chemical potential of LiBr	J/g	$\mu_{\text{LiBr}} = \text{LiBrSSCus}(T_c, X, P)$
Volume	m ³ /kg	$v = \text{LiBrSSCv}(T_c, X)$
Entropy	J/g-K	$s = \text{LiBrSSCs}(T_c, X, P)$ or $s_{\text{sat}} = \text{LiBrSSCs}(T_c, X)$
Saturation pressure	kPa	$P_{\text{sat}} = \text{LiBrSSCp}(T_c, X)$
Saturation temperature	°C	$T_{\text{sat}} = \text{LiBrSSCT}(P, X)$
Saturation mass fraction	-	$X_{\text{sat}} = \text{LiBrSSCX}(T_c, P)$
Crystallization temperature	°C	$T_{\text{cryst}} = \text{LiBrSSCTCryst}(X)$
Index of refraction	-	$N = \text{LiBrSSCRefIndex}(T_c, X)$
Procedures		
Partial mass Gibbs function	J/g	CALL LiBrSSCpart_g(Tc, X, P : g, dgdx, mu_w, mu_s)
Partial mass enthalpy	J/g	CALL LiBrSSCpart_h(Tc, X, P : h, dhdx, h_w, h_s)
Partial mass entropy	J/g-K	CALL LiBrSSCpart_s(Tc, X, P : s, dsdx, s_w, s_s)
Partial mass volume	m ³ /kg	CALL LiBrSSCpart_v(Tc, X : v, dvdx, v_w, v_s)
Flashing process	**	CALL LiBrSSCflash(h, P, x_in : q, T, x, hl, hv)
** - See details on units in procedure description Input Units: Tc - °C, X – mass fraction of LiBr, P – kPa Overloading – LiBrSSCCp, LiBrSSCCh, LiBrSSCCs all employ overloading such that if you do not input a value for pressure, the saturation pressure is assumed.		

There is also a set of functions listed in Table 2 that can call the routines in LiBrSSC.dll using the units set in EES with the \$UnitSystem directive of the Unit System dialog. These functions simply call the appropriate routine in Table 1, converting units as needed.

Table 2. Summary of LiBrSSC Helper Functions

Function	Example
Thermal conductivity	$k = \text{Cond_LiBrSSC}(T,X)$
Dynamic viscosity	$\mu = \text{Visc_LiBrSSC}(T,X)$
Specific heat	$c_p = \text{Cp_LiBrSSC}(T,X)$
Enthalpy	$h = \text{h_LiBrSSC}(T,X)$
Volume	$v = \text{v_LiBrSSC}(T,X)$
Entropy	$s = \text{s_LiBrSSC}(T,X)$
Saturation pressure	$P_{\text{sat}} = \text{Psat_LiBrSSC}(T,X)$
Saturation temperature	$T_{\text{sat}} = \text{Tsat_LiBrSSC}(P,X)$
Saturation mass fraction	$x = \text{xsat_LiBrSSC}(T,P)$
Crystallization temperature	$T_{\text{cryst}} = \text{Tcryst_LiBrSSC}(X)$
Flash calculation	Call $\text{Flash_LiBrSSC}(h,P,x;Q,T)$
The units of the properties for these functions are as selected with the \$UnitSystem Directive or the Unit System dialog. The units of properties are converted as needed to the unit system required by the LiBrSSC routine in Table 1.	

Transport Properties

The transport property correlations included were derived from an examination of available data. This was done as part of the SSC efforts but was unpublished [1]. Details of the correlations are summarized here

Viscosity

$$\ln \mu = A_0 + A_1 X^2 + \frac{B_0}{T} + \frac{B_1 X^2}{T} + \frac{C_0}{T^2} + \frac{C_1 X^2}{T^2}$$

where the units are μ (cP), T (K), X (mass fraction LiBr) and the constants are

$$\begin{aligned} A_0 &= -2.3212641667148 & A_1 &= 3.190587778753 \\ B_0 &= -609.44957160372 & B_1 &= 963.16370163469 \\ C_0 &= 372994.85578423 & C_1 &= -35211.99698739 \end{aligned}$$

This equation yields a R^2 value of 0.984073 across all of the data sets used. Example calculation: $T = 25^\circ\text{C}$ (298.15 K), $X = 0.5 \rightarrow \mu = 3.807$ cP.

Thermal Conductivity

$$k = A_0 + A_1X + B_0T + B_1TX + C_0T^2 + C_1T^2X + D_0T^3 + D_1T^3X$$

where $k = \text{W/m-K}$, $T = \text{K}$ & $X = \text{mass fraction LiBr}$

$$A_0 = -0.880453887702949$$

$$B_0 = 0.00898659269884302$$

$$C_0 = -1.55427759660091E-05$$

$$D_0 = 7.3203107999836E-09$$

$$A_1 = 0.883985046484968$$

$$B_1 = -0.007666522227789178$$

$$C_1 = 1.38873506415764E-05$$

$$D_1 = -6.31953452062666E-09$$

Our “best fit” produced an R^2 value of 0.9844 and the most well behaved curve over a broad range of the independent parameters. There were equations that had higher R^2 values but the one shown above had the best combination of properties. Example calculation: $T = 25^\circ\text{C}$ (298.15 K), $X = 0.5 \rightarrow k = 0.444 \text{ W/m-K}$.

Index of Refraction

The index of refraction of aqueous lithium bromide can be calculated from the correlation of Bostick et al. [2]

$$N = N_1x^2 + N_2x + N_3T + N_4$$

where

i	N_i
1	0.0000241
2	0.00108
3	-0.000106
4	1.3348

Units: $T - ^\circ\text{C}$, $x - \text{mass fraction LiBr in \%}$

Crystallization Temperature

The crystallization temperature is calculated from a curve fit to the data of Boryta [3].

$$x = A_0 + A_1T + A_2T^2$$

i	A_i		
	65.05 < x < 71.91	57.08 < x < 65.05	48.47 < x < 57.08
0	62.63716	56.95202	56.55952
1	0.04810823	0.05205944	0.2337275
2	0.00024301	0.00346278	0.00141297

Units: $T - ^\circ\text{C}$, $x - \text{mass fraction LiBr in \%}$

Thermodynamic Properties

The thermodynamic properties include volume, enthalpy, specific heat, entropy and chemical potential as well as the saturation properties temperature and pressure. All of these properties are derived from a Gibbs function fitted to a broad set of data for the mixture. The advantage of this approach is that any thermodynamic property of interest can be easily derived from the Gibbs function. And a corollary is that all of the derived properties will be

thermodynamically consistent (up to the precision of the calculation). The details of the Gibbs function are available in the literature [4, 5]. It provides excellent fidelity with the available data over the full concentration range from pure water up to crystallization and from 0 – 300°C.

Enthalpy of Aqueous Lithium Bromide

$$h = \text{LiBrSSCh}(T,x) \quad \text{or} \quad h = \text{LiBrSSCh}(T,x,P)$$

In general, we expect three independent properties to be required to specify state for a binary mixture such as aqueous lithium bromide. However, because the pressure effect is usually small, it is often omitted from property correlations for this mixture. The SSC routines retain and calculate pressure effects. However, to simplify routine use where the pressure effects can be ignored, the SSC enthalpy routine has an overload feature which calculates (and uses) the saturation pressure for cases where the user does not input a pressure value. Example calculation: $T = 25^\circ\text{C}$ (298.15K), $X = 0.5 \rightarrow h = 52.92 \text{ J/g}$.

Entropy of Aqueous Lithium Bromide

$$s = \text{LiBrSSCs}(T,x) \quad \text{or} \quad s = \text{LiBrSSCs}(T,x,P)$$

Example calculation: $T = 25^\circ\text{C}$ (298.15K), $X = 0.5 \rightarrow s = 0.1853 \text{ J/g-K}$.

Specific Heat of Aqueous Lithium Bromide

$$cp = \text{LiBrSSCcp}(T,x) \quad \text{or} \quad cp = \text{LiBrSSCcp}(T,x,P)$$

Example calculation: $T = 25^\circ\text{C}$ (298.15K), $X = 0.5 \rightarrow cp = 2.151 \text{ J/g-K}$.

Specific Volume of Aqueous Lithium Bromide

$$v = \text{LiBrSSCv}(T,x)$$

Example calculation: $T = 25^\circ\text{C}$ (298.15K), $X = 0.5 \rightarrow v = 0.0006523 \text{ m}^3/\text{kg}$

Chemical Potential in Aqueous Lithium Bromide

CALL LiBrSSCpart_g(Tc, X, P : g, dgdX, mu_w, mu_s)

$\mu_w = \text{LiBrSSCuw}(Tc,X, P)$

$\mu_s = \text{LiBrSSCus}(Tc,X, P)$

$$g_w = \mu_w = g - x \left(\frac{\partial g}{\partial x} \right)_{p,T}$$

$$g_s = \mu_s = g + (100 - x) \left(\frac{\partial g}{\partial x} \right)_{p,T}$$

Example calculation: $T = 25^\circ\text{C}$ (298.15K), $X = 0.5 \text{ LiBr}$, $P = 0.8071 \text{ kPa} \rightarrow g = -2.337 \text{ J/g}$, $dg/dx = 3.785 \text{ J/g}$, $g_w = -191.6 \text{ J/g}$, $g_s = 186.9 \text{ J/g}$.

One of the aspects of partial properties is that you can sum them up to obtain the mixture property as

$$g = \frac{(100 - x)g_w + xg_s}{100}$$

Partial Enthalpy in Aqueous Lithium Bromide

CALL LiBrSSCpart_h(Tc, X, P : h, dhdx, h_w, h_s)

$$h_w = h - x \left(\frac{\partial h}{\partial x} \right)_{p,T}$$
$$h_s = h + (100 - x) \left(\frac{\partial h}{\partial x} \right)_{p,T}$$

Example calculation: T = 25°C (298.15K), X = 0.5 LiBr, P = 0.8071 kPa → h = 52.92 J/g, dh/dx=1.944 J/g, h_w = -44.25 J/g, h_s = 150.1 J/g.

One of the aspects of partial properties is that you can sum them up to obtain the mixture property as

$$h = \frac{(100 - x)h_w + xh_s}{100}$$

Partial Entropy in Aqueous Lithium Bromide

CALL LiBrSSCpart_s(Tc, X, P : s, dsdx, s_w, s_s)

$$s_w = s - x \left(\frac{\partial s}{\partial x} \right)_{p,T}$$
$$s_s = s + (100 - x) \left(\frac{\partial s}{\partial x} \right)_{p,T}$$

Example calculation: T = 25°C (298.15K), X = 50 % LiBr, P = 0.8071 kPa → s = 0.1853 J/g-K, ds/dx=-0.006176 J/g-K, h_w = 0.4942 J/g-K, s_s = -0.1235 J/g-K.

One of the aspects of partial properties is that you can sum them up to obtain the mixture property as

$$s = \frac{(100 - x)s_w + xs_s}{100}$$

Partial Volume in Aqueous Lithium Bromide

CALL LiBrSSCpart_v(Tc, X : v, dvdx, v_w, v_s)

$$v_w = v - x \left(\frac{\partial v}{\partial x} \right)_{p,T}$$
$$v_s = v + (100 - x) \left(\frac{\partial v}{\partial x} \right)_{p,T}$$

Example calculation: T = 25°C (298.15K), X = 0.5 LiBr → v = 0.6523 cm³/g, dv/dx=-0.006976 cm³/g, v_w = 1.001 cm³/g, v_s = 0.3033 cm³/g.

One of the aspects of partial properties is that you can sum them up to obtain the mixture property as

$$s = \frac{(100 - x)s_w + xs_s}{100}$$

Saturation Properties of Aqueous Lithium Bromide

$$\begin{aligned}P_{\text{sat}} &= \text{LiBrSSCp}(T,x) \\T_{\text{sat}} &= \text{LiBrSSCT}(P,X) \\X_{\text{sat}} &= \text{LiBrSSCX}(Tc,P)\end{aligned}$$

Example calculation: $T = 25\text{C}$, $X = 0.5 \rightarrow P = 0.8071 \text{ kPa}$

Flashing of Aqueous Lithium bromide

CALL LiBrSSCflash(h, P, x_in : q, T, x, hl, hv)

This is a utility routine to automate the mass and energy balances involved in flashing through a valve or other pressure restriction. It assumes an adiabatic process. Inputs are enthalpy (h), LiBr mass fraction and the pressure at the outlet of the restriction. Outputs are the vapor quality (q), temperature (T), liquid mass fraction (x), liquid enthalpy (hl) and vapor enthalpy (hv).

Example calculation: $h = 74.54 \text{ J/g}$, $P = 0.5 \text{ kPa}$, $x_{\text{in}} = 0.5 \rightarrow q = 0.0137$, $T = 18.55^\circ\text{C}$, $x_l = 0.507$, $h_l = 40.66 \text{ J/g}$, $h_v = 2536 \text{ J/g}$.

Note: The overall mass, LiBr mass and energy balances are all satisfied.

References

1. SSC, *Transport Property Data for Aqueous Lithium Bromide*, in *SSC Unpublished Report* 1998.
2. Bostick, D.A., Klatt, L.N., Perez-Blanco, H., *Fiber optics refractometer for absorption machines*, 1987.
3. Boryta, D.A., *Solubility of Lithium Bromide in Water Between -50°C and 100°C (45 to 70% Lithium Bromide)*. *J. Chem. Eng. Data*,, 1970. **15**(1): p. 142-144.
4. Yuan, Z. and K.E. Herold, *Thermodynamic properties of aqueous lithium bromide using a multiproperty free energy correlation*. *HVAC&R Research*, 2005. **11**(3): p. 377-393.
5. Yuan, Z. and K.E. Herold, *Specific heat measurements on aqueous lithium bromide*. *HVAC&R Research*, 2005. **11**(3): p. 361-375.