

# Modelica Modeling of Thermodynamic Properties of LiBr-H<sub>2</sub>O Solutions

Kunfeng Sun \*

School of Energy and Environment, Zhongyuan University of Technology, Zhengzhou, China

\*Corresponding author: Kunfeng Sun (Email: skf0558@sina.com)

**Abstract:** Absorption refrigeration system is one of the basic refrigeration systems, with LiBr-H<sub>2</sub>O solution being the most common working fluid. In order to perform thermodynamic design and analysis on the absorption refrigeration cycle, it is essential to develop a program to calculate the thermodynamic properties of the solution. Modelica is the most promising digital twin modeling language and has been widely used in heat flow system modeling. In this study, a new interface library for calculating the thermophysical properties of LiBr-H<sub>2</sub>O solution is introduced. This library can calculate the vapor pressure, solution temperature, enthalpy, entropy, mass concentration, etc., as well as dynamic viscosity, thermal conductivity, surface tension coefficient, and other heat transfer or thermodynamics characteristic parameters. It enables researchers to easily modeling and analyze complex LiBr-H<sub>2</sub>O absorption refrigeration cycles in Modelica within specific temperature and concentration ranges.

**Keywords:** Thermodynamic properties, LiBr-H<sub>2</sub>O, Solutions, Modelica.

## 1. Introduction

With the development of the world economy, human beings are facing increasingly severe energy shortages and resources crises. Therefore, research on the utilization of renewable energy such as solar energy, geothermal energy, and low-grade energy such as industrial waste heat is receiving increasing attention. The unique advantage of absorption refrigeration, which can directly use low-grade heat sources to drive and does not use working fluids such as CFCs that damage the ozone layer, has been widely recognized [1].

Absorption refrigeration system is one of the fundamental refrigeration systems, in which LiBr-H<sub>2</sub>O Solutions being the most common working fluid. In order to perform thermodynamic calculations and analysis on the absorption refrigeration cycle, it is essential to develop a program to calculate the thermodynamic properties of the solution. Modelica language is currently the most promising digital twin development language. When modeling thermal-fluid systems, the Modelica standard library provides many medium models, but they may not be sufficient for many applications.

Absorption refrigeration system is one of the fundamental refrigeration systems. Currently, LiBr-H<sub>2</sub>O and NH<sub>3</sub>-H<sub>2</sub>O are widely used as working fluids in absorption refrigeration. Among them, NH<sub>3</sub>-H<sub>2</sub>O is limited in many applications due to its strong odor and toxicity, which compromises its safety.

On the other hand, LiBr-H<sub>2</sub>O primarily uses water as the refrigerant and can be used as long as the evaporation temperature is not lower than 5 °C. In order to perform thermodynamic calculations and analysis on the absorption refrigeration cycle, it is essential to develop a program to calculate the thermodynamic properties of the solution. Many researchers have conducted data fitting on the experimental data of lithium bromide-water solution's thermophysical properties and obtained equations for major property parameters [2]. ASHRAE has also provided equilibrium equations for lithium bromide-water solution [3].

Some scholars have developed software for calculating thermophysical properties using computer languages such as C, VB, Python, and Fortran etc. [4-6]]. These software packages generally include relationships between enthalpy, temperature, and concentration as the main parameters. However, developing refrigeration models in these languages is challenging, especially for complex models.

The release of Modelica is a significant event in the history of digital modeling technology development, marking the transition of these techniques from component-level to system-level in multiple disciplines and fields. After more than 20 years of development, Modelica has been widely applied in various industries such as aerospace, vehicles, energy, education, etc. Modelica combines the advantages of multiple modeling languages. Modelica is a high-level declarative language for describing mathematical behavior. It can easily describe the working characteristics of different engineering components, and at the same time, it can form complex systems of components [7, 8].

Modelica provides broad technical support for various modeling forms, including object-oriented and noncausal declarative modeling. Importantly, Modelica has an open language standard design, and its language specification is freely available. Additionally, there is an open-source IDE called OpenModelica. With its comprehensive features, Modelica has become the most promising digital twin development language and has the potential to become the de facto international standard for system simulation in the future.

Due to various advantages mentioned above, Modelica has been increasingly applied in the field of heat flow system modeling. When modeling a thermal fluid system, a fundamental question is whether a Modelica model can be obtained for calculating the properties of the working fluid. The Modelica standard library provides many medium models, but it is not sufficient in many specific applications, such as obtaining the thermodynamic properties of the working fluid solution for thermal calculation and analysis of absorption refrigeration cycles, which is essential and

challenging. To address this issue, the author of this article developed the Lithium Bromide solution thermodynamic property library for calculating the thermophysical properties of lithium bromide aqueous solutions. This library allows researchers to easily and conveniently model, calculate, and analyze complex absorption refrigeration cycles in Modelica within specific temperature and concentration ranges.

## 2. Framework of Library

The thermophysical property library consists of five main parts: LiBr, Saturation, Transports, tools and Example.

The framework of the thermophysical properties calculation library for LiBr-H<sub>2</sub>O solution is shown in Figure 1.

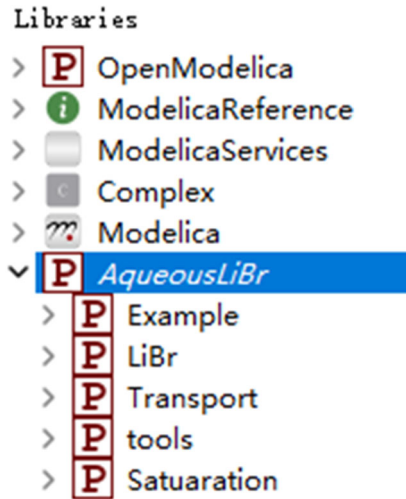


Figure 1. LiBr-H<sub>2</sub>O solution library framework

## 3. Thermal Properties

### 3.1. Enthalpy of LiBr-H<sub>2</sub>O Solution

The main calculations in absorption refrigeration models are the enthalpy difference, temperature difference, pressure difference, and concentration difference of each component. The enthalpy equation for the LiBr-H<sub>2</sub>O solution can be found in many different studies. In this work, ASHRAE handbook's enthalpy equation was used to develop the code. According to the ASHRAE handbook, enthalpy equation is expressed as following [3]:

$$h = \sum_0^4 A_n (100x)^n + T \sum_0^4 B_n (100x)^n + T^2 \sum_0^4 C_n (100x)^n \quad (1)$$

(15°C < T < 165°C, 0.4 < x < 0.7)

Where, h is enthalpy in kJ/kg, x is mass concentration and t is the solution temperature in °C, A(n), B(n) and C(n) are constants respectively.

Based on this code, a diagram of the relationship between solution concentration, solution temperature, and enthalpy can be generated, as shown in Figure 2.

### 3.2. Entropy of LiBr-H<sub>2</sub>O Solution

Just like calculating enthalpy, there are many equations for calculating the entropy of LiBr-H<sub>2</sub>O solution. Here, the equation in reference [9].

$$S = \sum_{i=0}^3 \sum_{j=0}^3 B_{ij} (100x)^j T^i \quad (2)$$

(40°C < T < 210°C, 0.4 < x < 0.65)

Where S is solution entropy in kJ/(kg.K). B are constants.

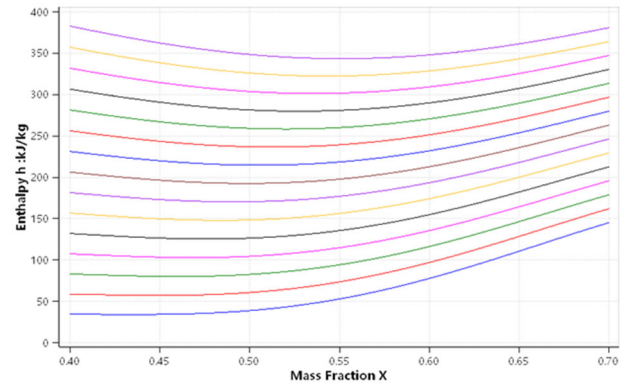


Figure 2. The LiBr-H<sub>2</sub>O solution enthalpy-concentration-temperature diagram

Other parameter calculations can refer to the functions in Table 1 and be calculated based on the corresponding functions.

Table 1. The Thermal Properties Functions

| Number | Name   | Function  | Scope                             |
|--------|--------|---|-----------------------------------|
| 1      | H_tx   | Determine enthalpy given temperature and concentration    | 15°C < T < 165°C, 0.40 < x < 0.70 |
| 2      | H_tp   | Determine enthalpy given temperature and pressure         | 15°C < T < 165°C, 0.25 < P < 200  |
| 3      | S_tx   | Determine entropy given temperature and pressure          | 40°C < T < 210°C, 0.40 < x < 0.65 |
| 4      | T_xp   | Determine temperature given concentration and pressure    | 0.25 < P < 200, 0.45 < x < 0.75   |
| 5      | P_xt   | Determine pressure given temperature and concentration    | 15°C < T < 165°C, 0.40 < x < 0.70 |
| 6      | X_tp   | Determine concentration given temperature and pressure    | 15°C < T < 165°C, 0.25 < P < 200  |
| 7      | T_hx   | Determine temperature given enthalpy and concentration    | 0.40 < x < 0.70                   |
| 8      | Hcn_h  | Enthalpy conversion function                              |                                   |
| 9      | Tcry_x | Determine crystallization temperature given concentration | 0.55 < x < 0.65                   |

## 4. Other Parameters

### 4.1. Transport Parameters

When calculating the heat exchanger model, the transport parameters are used, including specific heat capacity at constant-pressure, dynamic viscosity, thermal conductivity, and surface tension coefficient. Several references [5,9] have conducted fittings on these heat transfer parameters of lithium bromide-water solution, resulting in different fitting

equations. The computational accuracy of these equations is similar, with only slight variations in their applicable ranges. In this article, the following formula is selected.

Thermal conductivity:

$$k = \sum_{i=0}^3 A_i T^i + \sum_{i=1}^3 B_i x^i \quad (3)$$

Dynamic viscosity:

$$\eta = \sum_{i=0}^4 A_i x^i + T \sum_{i=0}^4 B_i x^i + T^2 \sum_{i=0}^4 C_i x^i \quad (4)$$

Surface tension coefficient:

$$\sigma = \sum_{i=0}^3 A_i T^i + \sum_{i=1}^3 B_i x^i \quad (5)$$

Where, k is thermal conductivity W/(m.K);

$\eta$  is Dynamic viscosity Pa.s;

$\sigma$  is surface tension coefficient N/m;

A, B is constants.

Figure 3 illustrates the relationship curve between thermal

conductivity and solution concentration at 40 °C.

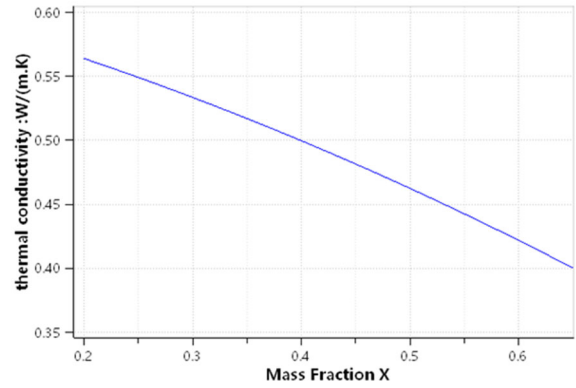


Figure 3. conductivity-x diagram at 40°C

Transport parameters calculations can refer to the functions in Table 2 and be calculated based on the corresponding functions.

Table 2. Transport Properties Functions

| Number | Name       | Function  | Scope                        |
|--------|------------|---|------------------------------|
| 1      | Density_tx | Determine density given temperature and concentration                     | 0°C<T<200°C,<br>0.40<X<0.70  |
| 2      | Cp_tx      | Determine specific heat capacity given temperature and concentration      | 20°C<T<190°C,<br>0.30<X<0.65 |
| 3      | Visc_tx    | Determine Dynamic viscosity given temperature and concentration           | 0°C<T<200°C,<br>0.45<X<0.65  |
| 4      | Cond_tx    | Determine thermal conductivity given temperature and concentration        | 20°C<T<200°C,<br>0.30<X<0.65 |
| 5      | Sigma_tx   | Determine Surface tension coefficient given temperature and concentration | 20°C<T<130°C,<br>0.40<X<0.70 |

## 4.2. Saturation Parameters

The calculation of saturation parameters requires the use of some physical properties of water vapor. There are two methods that can be used here. One is to directly call the water vapor physical properties package in the Modelica Media library, which has high calculation accuracy. The second

method is to separately use some empirical formulas in the range of 0-200 °C for calculation. This calculation library uses several simple formulas provided in reference[10], which are simple, fast, and can ensure accuracy, I won't list them all here anymore. Please refer to Table 3 for specific calculation functions.

Table 3. Saturation Parameters Functions

| Number | Name     | Function  | Scope                  |
|--------|----------|---|------------------------|
| 1      | Tsat_DtX | Determine Saturation temperature given dew temperature and concentration          | 0°C<T<200°C,<br>X<0.70 |
| 2      | Tsat_Dpx | Determine Saturation temperature given dew pressure and concentration             |                        |
| 3      | Xsat_Pdt | Determine Saturation concentration given dew pressure and solution temperature    |                        |
| 4      | Xsat_Dtt | Determine Saturation concentration given dew temperature and solution temperature |                        |
| 5      | hsat_tx  | Determine Saturation enthalpy given solution temperature and concentration        |                        |

## 4.3. Derived Parameter

There is not a direct equation for concentration in ASHRAE handbook. For example, given the pressure and

concentration, there is no equation that can directly calculate the solution temperature. In order to calculate the solution temperature, it is necessary to solve a nonlinear equation.

In this study, the nonlinear equation solving function

provided by Modelica is called, which uses the brent method to solve the nonlinear equation.

The sample code is as follows:

```
function X_tp
  extends Modelica.Icons.Function;
  input Real T;
  input Real p;
  output Real x;
protected
  Real x1 = 0.4;
  Real x2 = 0.7;
  Real tolerance = 100 * Modelica.Constants.eps;
algorithm
  x:=Modelica.Math.Nonlinear.solveOneNonlinearEquation
    ( function AqueousLiBr.tools.fun(T = T, p = p),
      x1,
      x2,
      tolerance);
end X_tp;
```

Figure 4 is the pressure-concentration-enthalpy diagram calculated by solving the nonlinear equations.

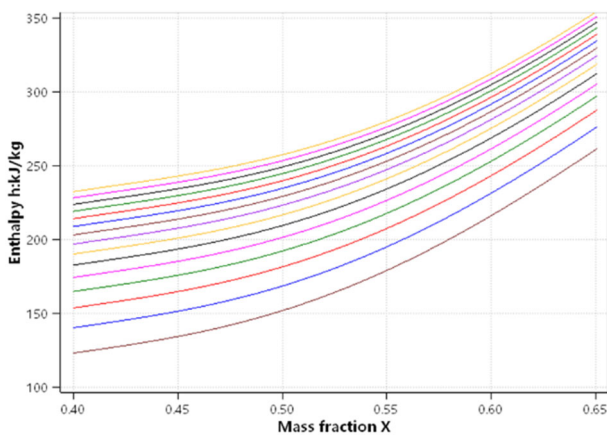


Figure 4. The enthalpy-concentration-pressure diagram

## 5. Conclusion

A thermophysical model library for LiBr-H<sub>2</sub>O solution was established using Modelica., Several parameters were explained in detail, and the calculation formulas for transport parameters and saturation parameter calculation functions

were provided. The tables explain the usage methods and limitations of LiBr-H<sub>2</sub>O solution. This library can conveniently calculate the thermophysical parameters of absorption refrigeration system cycles, meet the accuracy requirements of engineering calculations, and it can intuitively and conveniently draw parameter lines in the modelica.

## References

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