Effect of temperature and mole fraction on viscosity and thermal conductivity of water and ethanol mixture

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Abstract. The viscosity and thermal conductivity of the mixture as a heat exchange medium are the main factors affecting the heat transfer performance. In this paper, the mixture of water and ethanol is used as the research object. The viscosity and thermal conductivity of gas and liquid are calculated by various methods. Combined with the experimental data, the variation law with temperature and mole fraction is analysed, and the difference of different calculation methods is compared. When calculating the viscosity of water and ethanol mixture, the Teja and Rice method and the Jouyban and Acree method are suitable for different temperature ranges. The Jamieson method is more practical than the Baroncin method, when calculating the thermal conductivity. Finally, the calculation results are applied to an ejector refrigeration system calculation program, and it is found that the viscosity and thermal conductivity of the heat exchange medium have an important influence on the accuracy of the system performance calculation.

1. Introduction

In industries related to heat transfer, the operation of the heat exchanger directly affects the efficiency of the heat exchange system. Therefore, efficient heat transfer is the key technology to achieve effective energy use, and is an effective means to achieve energy conservation and emission reduction. In the heat exchanger, the viscosity and thermal conductivity of the heat exchange medium are the main factors affecting the heat transfer performance, and are the very important factors in the design of the heat exchanger [1].

In recent years, through experimental research and theoretical analysis, the viscosity and thermal conductivity of pure materials have a more practical calculation method [2]. However, the calculation method of the viscosity and thermal conductivity of the mixture has been ambiguous, and it is mostly determined by the experience of various industries [3]. Nowadays, more and more mixtures are used as heat exchange media in industrial production, so the determination of the physical properties of the mixture, especially the viscosity and thermal conductivity, is becoming more and more important [4].

In this paper, the mixture of water and ethanol is taken as the research object. The calculation methods of viscosity and thermal conductivity in gaseous and liquid state are introduced by comparison. The results are applied to a certain type of refrigeration system. It can be seen that the viscosity and thermal conductivity have an important influence on the actual heat transfer process.

2. Calculation method

For mixtures, the viscosity and thermal conductivities are calculated differently in both gaseous and liquid form. We study several computational methods and write calculation programs by C Language.
separately, and finally select several methods described below, these methods are more suitable for calculating water and ethanol related substances than other methods [1]. These methods are applicable to a variety of mixtures, ethanol and water mixtures are the subject of this study.

2.1. Viscosity of liquid mixture
By comparing the previous researches and the calculation method of the viscosity of liquid pure matter, this paper determines two calculation methods of the viscosity of liquid mixture.

Method of Teja and Rice requires the viscosity of ethanol and water at a certain conversion temperature [5], the core formulas is as follows:

\[ \ln(\eta_m e_m) = x_1 \ln(\eta_1 e_1) + x_2 \ln(\eta_2 e_2) \]
\[ \varepsilon = V^{2/3}/(TM)^{1/2} \]

Where \( V \) represents the molar volume, \( T \) is the absolute temperature, \( M \) is the relative molecular mass, \( x \) is the mole fractions of component, \( \eta \) is the viscosity, and the subscripts 1, 2 and \( m \) represent the two components of the mixture and the composition mixture, respectively.

Method of Jouyban and Acree can calculate various parameters of the mixture [1], and the formula for the viscosity is as follows:

\[ \ln\eta_m = x_1 \ln\eta_1 + x_2 \ln\eta_2 + A(x_1 x_2 / T) + B(x_1 x_2 (x_1 - x_2) / T) + C(x_1 x_2 (x_1 - x_2)^2 / T) \]

Where \( A, B, \) and \( C \) are coefficients calculated according to experimental parameters.

2.2. Thermal conductivity of liquid mixture
Method of Jamieson is the recommended method for the National Engineering Laboratory [1],

\[ \lambda_m = w_1 \lambda_1 + w_2 \lambda_2 - \alpha (\lambda_2 - \lambda_1) (1 - w_2^{1/2}) w_2 \]

Where \( \lambda \) is the thermal conductivity, \( w \) is the weight fraction. \( \alpha \) is an adjustable parameter that is set equal to unity if mixture data are unavailable for regression purposes.

Method of Baroncini was tested with over 600 datum points on 50 binary systems including those with highly polar components,

\[ \lambda_m = [x_1^2 A_1 + x_2^2 A_2 + 2.2 x_1 x_2 (A_1 / A_2)^{1/2}] (1 - T_r)^{0.38} / T_r^{1/6} \]

Where \( T_r \) is the reduced temperature and is converted from absolute temperature. The \( A \) parameters can be calculated from pure component thermal conductivities [1].

2.3. Viscosity of gas mixture
For method of TRAPP, the viscosity is determined by a combination of the techniques with appropriate mixing rules [1]. The viscosity of the mixture is given by a series of complex formulas, where the core formula is as follows,

\[ \eta_m - \eta_{m0} = F(\eta_R - \eta_{R0}) + \Delta \eta \]

Where \( R \) represents the reference fluid propane, the superscript \( o \) represents the low pressure state, and the coefficient \( F \) can be calculated from the parameters of two components.

When using the method of TRAPP, it is necessary to calculate the low-pressure state parameter of the pure substance in advance. At this time, the method of Chung is needed,

\[ \eta = 40.785 \left[ \omega (MT)^{1/2} / (V_c^{2/3} \Omega) \right] \]

Where \( \omega \) is the coefficient, which is detected by the literature, \( \Omega \) is viscosity collision integral from other equations, \( V_c \) is the critical volume.
2.4. Thermal conductivity of gas mixture
The calculation of the gas thermal conductivity is similar to the calculation of the viscosity, and the method of TRAPP is also adopted,
\[ \lambda_m - \lambda_m^0 = FX(\lambda_R - \lambda_R^0) \]  
(8)
Where F and X can be calculated from the parameters of two components, respectively.
The parameters of the low pressure state are calculated by the method of Eucken,
\[ \lambda^o = (1.32C_P^o + 3.741)\left(\frac{\eta^o}{M}\right) \]  
(9)
Where \(C_P^o\) is specific heat capacity in low pressure state.

According to the calculation needs, some places in this paper also use the calculation method provided by National Institute of Standards and Technology (NIST). The details of NIST method are not repeated here.

| Absolute temperature (K) | Experimental data | Jouyban and Acree method | Teja and Rice method |
|--------------------------|------------------|--------------------------|---------------------|
|                          | Viscosity (10^{-3}Pa.s) | Deviation (%) | Viscosity (10^{-3}Pa.s) | Deviation (%) |
| 373                      | 0.5337           | 0.5663                  | 6.1                 | 0.5548       | 4.0                |
| 363                      | 0.5516           | 0.6492                  | 17.7                | 0.6341       | 14.9               |
| 353                      | 0.5935           | 0.7513                  | 26.6                | 0.7319       | 23.3               |
| 343                      | 0.6916           | 0.8791                  | 27.1                | 0.8544       | 23.5               |
| 333                      | 0.7923           | 1.0414                  | 31.4                | 1.0105       | 27.5               |
| 323                      | 0.9587           | 1.2515                  | 30.5                | 1.2205       | 27.3               |
| 318                      | 1.1037           | 1.3804                  | 25.1                | 1.3432       | 21.7               |
| 313                      | 1.4442           | 1.5295                  | 5.9                 | 1.4955       | 3.6                |
| 308                      | 1.6249           | 1.7031                  | 4.8                 | 1.6690       | 2.7                |
| 303                      | 2.0666           | 1.9069                  | 7.7                 | 1.8511       | 10.4               |
| 298                      | 2.4236           | 2.1480                  | 11.4                | 2.0909       | 13.7               |
| 293                      | 3.0705           | 2.4362                  | 20.7                | 2.3764       | 22.6               |

3. Results and analysis
3.1. Properties with temperature
First, the viscosity and thermal conductivity of the gaseous and liquid phases of the water and ethanol mixture at different temperatures were calculated. A mixture of water and ethanol with an ethanol mole fraction of 0.316 is commonly used in the alcohol production industry [6, 7]. The ethanol mole fraction of the mixture that is analysed in this section was 0.316, because there is sufficient experimental data for comparative analysis.

It can be seen from Figure 1 that although the two calculation methods are different, the data curve trend consistency is quite high. Compared with the experimental data, the Teja and Rice method error is smaller than the Jouyban and Acree method when the temperature is higher than 308K, and the Jouyban and Acree method error is smaller when the temperature is lower than 308K. As can be seen from Table 1, compared with the experimental data [3, 8], the two methods have larger errors between 320K and 350K, but the errors are smaller in other temperature ranges. Other concentrations of mixtures also exhibit this trend, so in practical applications, the Teja and Rice method is used at higher temperatures and the Jouyban and Acree method is used at lower temperatures.
In Figure 2, the thermal conductivity calculated by the Baroncini method and the Jamieson method is similar with temperature, but the value of the Baroncini method is always higher than the Jamieson method. Because of the structural characteristics of the Jamieson method, when it is used to calculate pure water or pure ethanol, the calculation result is consistent with NIST. It can be seen from Figure 2 that the trend of two methods is similar when calculating pure matter, but the value of the Baroncini method is always higher than the Jamieson method, that is, higher than the NIST value. This is consistent with the difference between the two methods when determining the thermal conductivity of the mixture. Therefore, the Jamieson method is more practical than the Baroncini method.

Figure 3 and Figure 4 show the relationship between the properties of ethanol and water mixtures calculated by the TRAPP method and temperature. The viscosity and thermal conductivity of the gaseous mixture increase linearly with temperature.

3.2. Properties with mole fraction
For the viscosity of the liquid mixture, as shown in Figure 5, experimental data [9] and calculated data show a similar trend. As the mole fraction of ethanol increases, the viscosity first increases, reaching a maximum between the mole fractions of 0.2-0.3, and then continues to decrease. Under other temperature conditions, the trend is also the same. By comparing with the experimental data, it can be
found that the Jouyban and Acree method can reasonably show the tendency of the viscosity of the liquid mixture to change with the mole fraction.

For the liquid mixture thermal conductivity varies with the mole fraction, the two methods show a similar trend, in Figure 6, but the specific values are still different.

When the mixture is in a gaseous state, as shown in Figure 7 and Figure 8, the viscosity and thermal conductivity decrease as the mole fraction of ethanol increases, which is consistent with the theoretical analysis.

3.3. Refrigeration system application analysis

The scheme and working process of the ejector refrigeration system are shown in Figure 9. The refrigerant absorbs the heat of the heat fluid source in the generator and enters the ejector, which becomes the high speed mainstream of the ejector [10]. The other refrigerant, which exchange heat in the evaporator, is introduced into the ejector by the mainstream and becomes a secondary flow. After the mainstream and secondary flow are mixed and pressurized, they enter the condenser to exchange heat with ambient. Finally, the refrigerant enters the generator and the evaporator respectively to continue the working cycle [11].

In the production of alcohol, it is often necessary to obtain a mixture of water and ethanol of different mole fractions and temperatures. This paper attempts to apply the above-mentioned ejector
refrigeration system to the production process of alcohol, and to study the ejector refrigeration system through C language. Therefore, in the system designed in this paper, the fluid in the heat fluid source and the user are water and alcohol mixtures with high temperature, while the fluid in ambient is a low temperature water and alcohol mixture, the calculation process is shown in Figure 10.

![Figure 9. Scheme of an ejector refrigeration system.](image)

The performance of the heat exchanger plays an important role in the normal operation of the ejector refrigeration system [12], and the system includes three main heat exchangers, a generator, an evaporator and a condenser. The heat exchanger uses a plate heat exchange method that uses phase change heat. Heat exchanger calculation is the core of the calculation program of this system. The calculation of viscosity and thermal conductivity is the core content of heat exchanger calculation. Therefore, in the calculation program used in this paper, the influence of viscosity and thermal conductivity is highlighted.

![Figure 10. The ejector refrigeration calculation process after adding the viscosity and thermal conductivity calculation program.](image)

The different calculation methods of viscosity and thermal conductivity in this paper are respectively connected to the calculation program of the refrigeration system, and finally some results are shown in Table 2.

COP and the second law efficiency are important indicators for evaluating the refrigeration system [13]. From the results, it can be seen that using different methods to calculate the viscosity and thermal conductivity will make these indicators change greatly. Therefore, choosing the appropriate calculation method for viscosity and thermal conductivity is a key step in the calculation of the
refrigeration system. From the data in Table 2, the COP deviation calculated by Jamieson method, Eucken method and NIST is smallest.

| Viscosity method | Thermal conductivity method | Refrigeration system |
|------------------|-----------------------------|----------------------|
| Liquid           | Gaseous                     | Liquid               | Gaseous | COP | COP Deviation (%) | Efficiency |
| Experiment       | NIST                        | Jamieson             | Eucken  | 0.328 | 2.5 | 0.129 |
| Experiment       | NIST                        | Baroncini            | Eucken  | 0.334 | 4.4 | 0.131 |
| Experiment       | Chung                       | Baroncini            | NIST    | 0.351 | 9.7 | 0.133 |
| Experiment       | Chung                       | Jamieson             | NIST    | 0.354 | 10.6 | 0.135 |
| Jouyban Acree    | NIST                        | Jamieson             | Eucken  | 0.331 | 3.4 | 0.130 |
| Jouyban Acree    | Chung                       | Baroncini            | NIST    | 0.346 | 8.1 | 0.138 |

4. Conclusions
In this paper, the different methods of viscosity and thermal conductivity are programmed and the program is connected to an ejector refrigeration system calculation program. The following conclusions are obtained:

1. By comparing with experimental data, the calculation method determined in this paper can be used to analyze the viscosity and thermal conductivity of the mixture, and the tendency of viscosity and thermal conductivity to change with temperature and mole fraction are obtained. In particular, when calculating the viscosity of water and ethanol mixture, the Teja and Rice method and the Jouyban and Acree method are suitable for different temperature ranges. The Jamieson method is more practical than the Baroncini method, when calculating the thermal conductivity.

2. Combined with an ejector refrigeration system calculation program, it is found that different methods of viscosity and thermal conductivity will affect the performance of the refrigeration system, so the choice of the calculation method of viscosity and thermal conductivity is a key step in the design of the refrigeration system. The COP deviation calculated by Jamieson method, Eucken method and NIST is smallest.

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