The development of the equation and tables of dynamic viscosity of vapor mixture octafluoropropane and water

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Abstract. Dynamic viscosity of gaseous mixture of water vapor and octafluoropropane is calculated by means of Wilke’s equation and using the molecular-kinetic theory’s methods for all range of water vapor’s concentrations from 0 to 1 in the temperature range from 0 to 160 °C. The incorrectness of using in this case Wilke’s equation is shown. Preference is given to molecular-kinetic theory’s method, by means of which the analytical equation is obtained and tables of predicted values of mixture’s viscosity are calculated.

1. Introduction
In recent years the close attention is drawn to works related with research of a possibility of application of fluorocarbons, including octafluoropropane C₃F₈, as working fluid of power installations [1]. The possibility of using of mixture of octafluoropropane and water vapor in a power cycle is also considered.

In this case for calculations of heat transfer equipment, used in the power installations, information about thermophysical properties of these mixtures is necessary, including information about dynamic viscosity of a mixture. It is necessary to notice that any experimental data about this property of such a mixture in the literature do not exist. Therefore in this work the task of deriving of the data about dynamic viscosity of vapor phase of mixtures of octafluoropropane and water on the basis of the molecular theory or on the basis of methods of a similarity is considered.

2. Calculation of dynamic viscosity of mixture by a method of similarity
Dynamic viscosity of substances in a gas phase weakly depends on pressure. Therefore working out data for poorly studied mixtures it is possible to take into account only the dependence of viscosity from temperature. Such dependence for one of components of the considered system - rarefied water vapor, is well studied and presented in reference data [2]:

\[ \eta_v = \frac{100 \sqrt{T}}{\sum_{i} H_i / \bar{T}_i} \]  

(1)

where \( \bar{T} = T / 647,096 \), \( T \) – absolute temperature, K,
\( H_i \) – coefficients: \( H_1 = 1,67752 \); \( H_2 = 2,20462 \); \( H_3 = 0,6366564 \); \( H_4 = -0,241605 \)
For the second component – octafluoropropane, experimental data are not numerous and refer basically to liquid phase [3, 4]. Therefore in work [5] for the description of viscosity of the rarefied gas octafluoropropane the equation following from molecular-kinetic theory of properties of substances has been offered:

\[ \eta_U = 266.93 \times 10^{-4} \frac{\sqrt{M_U T}}{\sigma^2 \Omega^{2.2}}, \]

(2)

where \( \eta_U \) - viscosity, \( \mu \text{Pa.s} \), \( M_U \) – molar weight, \( \sigma \) – molecule diameter, nm, \( \Omega^{2.2} \) - an integral of collision.

As the function defining molecular interactions, the potential of Lennard-Jones (12-6) is used, which constants are defined as follows: \( \varepsilon / k_B = 266.35 K \), \( \sigma = 0.58 \text{ nm} \). The integral of collision thus can be computed by formula [6]:

\[ \Omega^{2.2} = [A \cdot (T^*)^{-B} + C \cdot \exp(-D T^*)] + E \cdot \exp(-F T^*)), \]

(3)

with \( T^* = T / (\varepsilon / k_B) \), and coefficients are equal: \( A = 1.16145; B = 0.14874; C = 0.52487; D = 0.77320; E = 2.16178; F = 2.43787 \)

Values of octafluoropropane viscosity calculated by equations (2, 3) are valid for temperature range from 273 K to 420 K.

For calculation of dynamic viscosity of mixtures of gases at known values of viscosity of components the Wilke’s method [7] may be used. In this method mixture viscosity is calculated via following relation:

\[ \eta_{cw} = \frac{x_1 \cdot \eta_w + x_2 \cdot \eta_U}{x_1 + x_2 \cdot \Phi_{12}}, \]

(4)

where \( x_1 \) и \( x_2 \) – mole fractions of water vapor and octafluoropropane, \( \eta_w \) and \( \eta_U \) - their viscosities;

\[ \Phi_{12} = \frac{[1 + (\eta_w / \eta_U)_{1/2} \cdot (M_U / M_w)]^{1/2}}{8 \cdot [1 + (M_w / M_U)]^{1/2}}, \]

(5)

\[ \Phi_{21} = \frac{M_w}{M_U} \cdot \frac{\eta_U}{\eta_w}, \]

(6)

here \( M_w \) and \( M_U \) - mole mass of water vapor and octafluoropropane.

Using equations (1)–(6), dynamic viscosity data of gas mixture of water vapor and octafluoropropane is calculated for all range of concentration of water vapor from 0 to 1 at temperature from 0 to 160 °C (Table A1). As an example, the dependence of mixture viscosity from a mass fraction of water vapor is presented in figure 1.

![Figure 1. Mixture viscosity at temperature 320 K](image-url)
3. Calculation of dynamic viscosity of vapor phase of mixture of octafluoropropane and water using molecular-kinetic theory

In molecular–kinetic theory of transport properties of mixtures of rarefied gases for the account of influence of interaction force between heterogeneous molecules on mixture viscosity, the following parameter is used:

\[
\eta_{12} = 266.93 \cdot 10^{-4} \frac{\sqrt{2M_W M_u T / (M_W + M_u)}}{\sigma_{12}^2 \cdot \Omega_{12}^{2.2}}
\]

(7)

where \( \sigma_{12} = 0.5 \cdot (\sigma_W + \sigma_U) \) and the integral of collision \( \Omega_{12}^{2.2} \) is calculated by equation (3) for reduced temperature \( T_{12}^* = T / (\varepsilon / \kappa_{B})_{12} \), with \((\varepsilon / \kappa_{B})_{12} = \sqrt{(\varepsilon / \kappa_{B})_W \cdot (\varepsilon / \kappa_{B})_U}\).

Molecular parameters of octafluoropropane \( \sigma_U \) and \((\varepsilon / \kappa_{B})_U\) are presented above, and for water vapor they have been obtained on the basis of the data \cite{2} for a range of temperatures from 273 K to 440 K. The received values of \( \sigma_W = 0.28 \) nm and \((\varepsilon / \kappa_{B})_W = 740.1\) K are well coordinated with the values defined in \cite{8} for potential of Lennard-Jones (12-6) in the region of high temperatures. Values of viscosity of water vapor, calculated by equation (2) with these parameters, are in agreement with the data of \cite{2} within ±2%.

At calculation of value of \( \eta_{12} \) it is necessary to take into account that one of mixture component – water vapor is the substance consisting of polar molecules with big enough dipole moment of 1.83 Debye, and molecules of the second component – octafluoropropane possess small dipole moment equal to 0.14 Debye. In this case the correction to molecular parameters of mixture is introduced and they are calculated as:

\[
\sigma_{12} = 0.5 \cdot (\sigma_W + \sigma_U) \cdot \xi^{-1/6}
\]

(8)

\[
(\varepsilon / \kappa_{B})_{12} = (\sqrt{\varepsilon / \kappa_{B}}_W \cdot (\varepsilon / \kappa_{B})_U) \cdot \xi^2
\]

\[
\xi = (1 + \frac{2}{2} \cdot a_n^* \cdot t_p^* \cdot \frac{\varepsilon / k_p}{\varepsilon / k_n})
\]

where \(a_n^*\) - the reduced polarizability of a non-polar molecule of octafluoropropane:

\[
a_n^* = a_n / \sigma_n;
\]

\(t_p^*\) - the reduced dipole moment of a molecule of water.

For the molecule of water value \( t_p^* = 1.2\) is well-known. Information about polarisation of octafluoropropane is absent. Therefore it is accepted on analogies to molecule \( \text{C}_3\text{H}_8\) having the same structure, \(a_n = 60 \cdot 10^{-25}\) cm³.

Character of dependence on temperature of the function \( \eta_{12} \), describing influence of intermolecular interaction of heterogeneous molecules on viscosity of a mixture, is presented in figure 2.

After \( \eta_{12} \) function definition, viscosity of gas mixture can be calculated on the equation of molecular–kinetic theory of transport properties, presented in \cite{9}:

\[
\eta_{cm}^{-1} = X_\eta \cdot \left[ \frac{1 + (Y_\eta / X_\eta)}{1 + Z_\eta} \right]
\]

(9)

here

\[
X_\eta = 2 \cdot X_1 \cdot X_2 + 2 \cdot X_1 / \eta_{12} + 2 \cdot X_2 / \eta_U
\]

(10)
Figure 2. Value $\eta_{12}$ for mixture

Figure 3 shows the dependency of mixture viscosity from the mass concentration of water vapor calculated using the equations (7) – (11) of molecular theory for temperature 330 K.

One can see the big difference of this dependence from the dependency calculated by the method of Wilke (figure 1). This difference is especially sharp in area of small concentration of water vapor. At calculation by method of Wilke viscosity of mixture at growth of concentration of water vapor in the beginning, till $g = 0.2$, exceeds viscosity of octafluoropropane in spite of the fact that viscosity of pure water vapor is less a little. After $g = 0.2$ it decreases rapidly to viscosity of water vapor. In calculations under the molecular theory at growth of concentration of water vapor viscosity of a mixture strongly enough and constantly decreases.

Such character of divergence of these dependencies remains the same at other temperatures. This difference of dependencies shows inapplicability of Wilke’s rule in this case, possibly due to the big difference of molecular masses of components ($M_u /M_W =10,4$). Therefore from two investigated methods of definition of mixture viscosity the preference is given to the method of molecular-kinetic
theory. The values of viscosity (Table B1) calculated with its use are presented in the form of equation convenient [10] for practical calculations:

\[ \eta_{cw} = \frac{a0 + a1 \cdot m + a2 \cdot T + a3 \cdot m^2 + a4 \cdot T^2 + a5 \cdot m \cdot T}{b0 + b1 \cdot m + b2 \cdot T + b3 \cdot m^2 + b4 \cdot T^2 + b5 \cdot m \cdot T}, \]

where \( m \) – mass fraction of water vapor, \( T, [K] \) – temperature.

Coefficients in equation (12) are presented in table 1.

**Table 1.** Coefficients of equation (12) for calculation of dynamic viscosity of octafluoropropane and water vapor mixture.

| Coefficients |  \\
|-------------|---------|---------|---------|---------|
| a           | b       |         |         |         |
| 0           | 7.340877256 | 1.00    |         |         |
| 1           | 4.019554423 | 2.680388726 |         |         |
| 2           | -0.02431659 | -0.00358484 |         |         |
| 3           | 0.947360854 | 0.079332648 |         |         |
| 4           | 4.74074e-05 | 4.6678e-06 |         |         |
| 5           | 0.051341623 | -0.00193208 |         |         |

4. Conclusion

Results of calculations show that the application of Wilke’s rule for determination of dynamic viscosity of mixture of components with very great difference in molecular mass of substances can gives insecure values in region of small mass fractions of light component. Molecular theory can gives more reliable data. The overall standard uncertainty of calculated values of viscosity of mixture of octafluoropropane and water vapor is estimated at 5 %

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Appendices

**Appendix A**

**Table A1.** Viscosity of gas mixture of octafluoropropane and water vapor calculated by Wilke’s formula.

| Mass fraction of water vapor | Dynamic viscosity, \( \mu Pa.s \) with temperature, °C |  \\
|-----------------------------|--------------------------------------------------------|
|                             | 0           | 50          | 100         | 150         |
| 0,0                         | 11.44       | 13.52       | 15.53       | 17.45       |
| 0,1                         | 11.68       | 13.80       | 15.92       | 17.99       |
| 0,2                         | 11.43       | 13.49       | 15.61       | 17.73       |
| 0,3                         | 11.04       | 13.03       | 15.12       | 17.23       |
| 0,4                         | 10.65       | 12.57       | 14.61       | 16.70       |
| 0,5                         | 10.29       | 12.13       | 14.12       | 16.19       |
| 0,6                         | 9.96        | 11.74       | 13.69       | 15.72       |
| 0,7                         | 9.66        | 11.39       | 13.29       | 15.29       |
| 0,8                         | 9.40        | 11.07       | 12.94       | 14.91       |
| 0,9                         | 9.16        | 10.79       | 12.62       | 14.56       |
| 1,0                         | 8.95        | 10.54       | 12.34       | 14.25       |
## Appendix B

**Table B1. Dynamic viscosity of mixture of octafluoropropane and water vapor.**

| Mass fraction of water vapor | Dynamic viscosity, µPa.s with temperature, K |
|-----------------------------|---------------------------------------------|
|                             | 280  | 290  | 300  | 310  | 320  | 330  | 340  | 350  | 360  | 370  | 380  | 390  | 400  | 410  | 420  |
| 0,00                        | 11.73| 12.15| 12.57| 12.98| 13.39| 13.8  | 14.21| 14.61| 15.01| 15.41| 15.8  | 16.19| 16.57| 16.95| 17.33|
| 0,10                        | 10.54| 10.91| 11.28| 11.66| 12.04| 12.43 | 12.82| 13.21| 13.6  | 14.0 | 14.39 | 14.79| 15.19| 15.58| 15.98|
| 0,20                        | 10.02| 10.36| 10.72| 11.08| 11.45| 11.82 | 12.2 | 12.58| 12.97| 13.36| 13.75 | 14.15| 14.54| 14.94| 15.34|
| 0,30                        | 9.73 | 10.07| 10.41| 10.76| 11.12| 11.48 | 11.86| 12.23| 12.61| 13.0 | 13.39 | 13.78 | 14.17| 14.57| 14.97|
| 0,40                        | 9.55 | 9.88 | 10.21| 10.56| 10.91| 11.27 | 11.64| 12.01| 12.39| 12.77| 13.15 | 13.54 | 13.93| 14.33| 14.73|
| 0,50                        | 9.43 | 9.75 | 10.08| 10.42| 10.77| 11.12 | 11.49| 11.85| 12.23| 12.61| 12.99 | 13.38 | 13.77| 14.16| 14.55|
| 0,60                        | 9.34 | 9.66 | 9.98 | 10.32| 10.66| 11.02 | 11.37| 11.74| 12.1 | 12.49| 12.87 | 13.25 | 13.64| 14.03| 14.43|
| 0,70                        | 9.27 | 9.59 | 9.91 | 10.24| 10.58| 10.93 | 11.29| 11.65| 12.02| 12.4 | 12.78 | 13.16 | 13.54| 13.93| 14.33|
| 0,80                        | 9.22 | 9.53 | 9.85 | 10.18| 10.52| 10.87 | 11.22| 11.59| 11.95| 12.33| 12.70 | 13.08 | 13.47| 13.86| 14.25|
| 0,90                        | 9.18 | 9.49 | 9.81 | 10.13| 10.47| 10.82 | 11.17| 11.53| 11.9 | 12.27| 12.64 | 13.02 | 13.41| 13.79| 14.18|
| 1,00                        | 9.15 | 9.45 | 9.77 | 10.1 | 10.43| 10.78 | 11.13| 11.49| 11.85| 12.22| 12.59 | 12.97 | 13.35| 13.74| 14.13|
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