Learning Objectives

1) Understand the different available methods for calculating thermodynamic properties of moist air.

2) Identify the differences between the ideal gas model and the real-gas model for evaluation of moist air thermodynamic properties.

3) Learn the state of the art models for the calculation of the transport properties of the pure components of the mixture moist air, dry air, and water.

4) Understand the differences between the new diagrams for viscosity and thermal conductivity for moist air compared with those from the current ASHRAE Handbook of Fundamentals.
1. Introduction

- **State of the art:** only two imprecise figures of transport properties of moist air, based on outdated equations, available in the current ASHRAE Handbook Ch. 1
- No ASHRAE Research Project was carried out on Transport Properties Research before RP-1767
- Extensive research on transport properties of dry air at NIST (2004)
- IAPWS sponsored significant research on transport properties of water and steam in the period from 1984 to 2014

- An unsolicited research proposal was written and submitted in 2015
- Proposal was reviewed, accepted and PMC was installed
- ASHRAE RP-1767 started on 1st of July, 2016, and will last up to 30th of June, 2018
2. Recent Transport Properties Research

- New correlations for the viscosity and the thermal conductivity of dry air were published by Lemmon and Jacobsen (2004)
- A new correlation for viscosity of H₂O were released as International Standard by IAPWS (2008) based on research by Huber et al. at NIST
- A new correlation for thermal conductivity of H₂O were released as International Standard by IAPWS (2011) based on research by Huber et al. at NIST
- Revised correlations for thermodynamic properties of moist air were developed within the ASHRAE Research Project RP-1485 (Herrmann et al., 2009)
- VW procedure to model viscosity and thermal conductivity for mixtures (Vesovic and Wakeham, 1989, 1991)
- Significant advancement in measuring moist air transport properties at higher pressures and temperatures resulting from research typical of the Compressed Air Energy Storage (CAES) process (final model can be used from 243 K to 1000 K and pressures to 40 MPa), European Union Project AA-CAES (2002-2006)

3. Algorithms for Moist Air Transport Properties

Calculation of Viscosity of Moist Air

- Viscosity of gas mixtures

\[ \eta_{\text{mix}}(T, \rho_m, \bar{x}) = \frac{H_{11} \cdots H_{1N} Y_1}{H_{N1} \cdots H_{NN} Y_N} + \kappa_{\text{mix}} \]

with

\[ Y_i = x_i \left( 1 + \sum_{j=1}^{N} \frac{m_j}{m_i + m_j} x_j \alpha_{ij} \bar{Z}_{ij} \rho_m \right) \]

\[ H_{ii} = \frac{x_i^2 \bar{Z}_{ii}}{\eta_i^0} + \sum_{j=1}^{N} \frac{x_i x_j \bar{Z}_{ij}}{m_i m_j} \left( \frac{20}{3} + \frac{4m_j}{m_i} A_{ij}^* \right) \]

\[ H_{ij} = -\frac{x_i x_j \bar{Z}_{ij}}{2A_{ij} \eta_i^0} \left( \frac{20}{3} - 4A_{ij}^* \right) \quad (i \neq j) \]

\[ \kappa_{\text{mix}} = \frac{16}{5\pi} \frac{15}{16} \rho_m^2 \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \alpha_{ij}^2 \eta_{ij}^0 \]

\[ \frac{1}{\alpha_{ij}} = \frac{1}{\alpha_{ij}^0} + \frac{1}{\alpha_{ij}^*} \]

1 Vesovic and Wakeham (1989)
• Contact value of the pseudo-radial distribution function for a pure component

\[ \bar{\chi}_i(T, \rho_m) = \beta \eta \left( \frac{\eta_i - \rho_m \alpha_{ii} \eta_i^0}{2 \rho_m^2 \alpha_{ii}^2 \eta_i^0} \right) \pm \beta \eta \left[ \left( \frac{\eta_i - \rho_m \alpha_{ii} \eta_i^0}{2 \rho_m^2 \alpha_{ii}^2 \eta_i^0} \right)^2 - \frac{1}{\beta \eta \rho_m^2 \alpha_{ii}^2} \right]^{1/2} \]

with \( \alpha_{ii} \) from

\[ \frac{\eta_i(T, \rho_m^*)}{\rho_m^* \alpha_{ii} \eta_i^0} = 1 + \frac{2}{\sqrt{\beta \eta}} \quad \text{and} \quad \left[ \frac{\partial \eta_i(T, \rho_m)}{\partial \rho_m} \right]_T = \frac{\eta_i(T, \rho_m^*)}{\rho_m^*}, \]

\[ \frac{1}{\beta \eta} = \frac{1}{4} + \frac{1}{16} \left( \frac{16}{5 \pi} \right) \quad \text{and} \quad \rho_m^* \text{ as switch-over density} \]

• Mixing rules

\[ \bar{\chi}_{ij} = 1 + \frac{2}{5} \sum_{k=1}^{N} x_k (\bar{\chi}_k - 1) + \frac{6}{5} (\bar{\chi}_i - 1)^{1/3} (\bar{\chi}_j - 1)^{1/3} \sum_{k=1}^{N} x_k (\bar{\chi}_k - 1)^{2/3} \]

\[ \alpha_{ij} = \frac{1}{8} \left( \alpha_{ii}^{1/3} + \alpha_{jj}^{1/3} \right)^3 \]

Calculation of Thermal Conductivity of Moist Air

• Thermal Conductivity of gas mixtures

\[ \lambda_{\text{mix}}(T, \rho_m, \bar{x}) = \lambda_{\text{mix}}(\text{mon})(T, \rho_m, \bar{x}) + \lambda_{\text{mix}}(\text{int})(T, \rho_m, \bar{x}) \]

\[ \lambda_{\text{mix}}(\text{int})(T, \rho_m, \bar{x}) = \sum_{i=1}^{N} \left[ \frac{\lambda_i^0 - \lambda_i^0(\text{mon})}{\bar{\chi}_{ii}} \right] \left[ 1 + \sum_{j=1}^{N} x_j \lambda_j^0(\text{mon}) \bar{\chi}_{ij} A_{ij}^* \right]^{-1} \]

Monatomic (mon) contribution

\[ \lambda_{\text{mix}}(\text{mon})(T, \rho_m, \bar{x}) = - \frac{1}{L_{N1} \cdots L_{NN}} Y_{N} \begin{bmatrix} Y_i \cdots Y_i \cdots Y_i \cdots Y_i \cr \vdots \cdots \vdots \cdots \vdots \cdots \vdots \cr L_{N1} \cdots L_{NN} \end{bmatrix} \begin{bmatrix} L_{11} \cdots L_{1N} \cr \vdots \cdots \vdots \cdots \vdots \cdots \vdots \cr L_{N1} \cdots L_{NN} \end{bmatrix} + \kappa_{\text{mix}} \]

\[ ^2 \text{Vesovic and Wakeham (1991)} \]
\[ Y_i = x_i \left[ 1 + \sum_{j=1}^{N} \frac{2m_im_j}{m_i + m_j} x_j \gamma_{ij} \lambda_{ij}(\text{mon}) \right] \]

\[ L_{ii} = \frac{x_i^2 \lambda_{ii}(\text{mon})}{\lambda_{ii}(\text{mon})} + \sum_{j \neq i}^{N} \frac{x_i x_j \lambda_{ij}}{2 \lambda_{ij}(\text{mon})(m_i + m_j)} \left( \frac{15}{2} m_i^2 + \frac{25}{4} m_j^2 - 3m_i^2 B_{ij}^* + 4m_i m_j A_{ij}^* \right) \]

\[ L_{ij} = -\frac{x_i x_j \lambda_{ij}}{2 \lambda_{ij}(\text{mon})(m_i + m_j)} \left( \frac{55}{4} - 3B_{ij}^* - 4A_{ij}^* \right) \quad (i \neq j) \]

\[ \kappa_{\text{mix}} = \frac{16}{5\pi} \frac{2m_i}{9} \frac{m_i m_j}{(m_i + m_j)^2} x_i x_j \gamma_{ij}^2 \lambda_{ij}^0(\text{mon}) \]

and

\[ \lambda_{ii}^0(\text{mon}) = \frac{5}{2} \left[ \frac{c_{m_i}^0(\text{mon})}{M_i} \right] \eta_i^0, \quad \lambda_{ij}^0(\text{mon}) = \frac{5}{2} \left[ \frac{c_{m_{ij}}^0(\text{mon})}{M_{ij}} \right] \eta_{ij}^0 \]

- Contact value of the pseudo-radial distribution function for a pure component

\[ \lambda(T, \rho_m) = \beta_\lambda \left[ \lambda_i - \rho_m \gamma_{ii} \lambda_{ii}^0(\text{mon}) \right] \pm \beta_\lambda \left[ \frac{\lambda_i - \rho_m \gamma_{ii} \lambda_{ii}^0(\text{mon})}{2 \rho_m \gamma_{ii}^2 \lambda_{ii}^0(\text{mon})} \right]^{1/2} \]

with \( \gamma_{ii} \) from

\[ \frac{\lambda_i(T, \rho_m^*)}{\rho_m \gamma_{ii} \lambda_{ii}^0(\text{mon})} = 1 + \frac{2}{\sqrt{\beta_\lambda}} \left[ \frac{\lambda_i^0(\text{mon})}{\lambda_i^0(\text{mon})} \right]^{1/2} \quad \text{and} \quad \left[ \frac{\partial \lambda_i(T, \rho_m)}{\partial \rho_m} \right]_T = \frac{\lambda_i(T, \rho_m^*)}{\rho_m^*} \]

\[ \frac{1}{\beta_\lambda} = \frac{1}{4} + \left( \frac{16}{5\pi} \right) \frac{5}{18} \quad \text{and} \quad \rho_m^* \text{ as switch-over density} \]

- Mixing rules

\[ \lambda_{ij} = 1 + \frac{2}{5} \sum_{k=1}^{N} x_k \left( \lambda_{kk} - 1 \right) \]

\[ \gamma_{ij} = \frac{1}{8} \left( \gamma_{ii}^{1/3} + \gamma_{jj}^{1/3} \right)^3 \]
Implementation of VW Mixing Models for Moist Air

- Treatment of critical enhancement for pure components
  \[ \eta_i(T, \rho_m) = \eta_{i,\text{total}}(T, \rho_m) - \eta_i^C(T, \rho_m) \]
  \[ \lambda_i(T, \rho_m) = \lambda_{i,\text{total}}(T, \rho_m) - \lambda_i^C(T, \rho_m) \]
  - critical enhancement subtracted from total value for pure fluid
  - performed for water only, since dry air far away from critical point
  \[ \lambda_{\text{mix,total}}(T, \rho_m) = \lambda_{\text{mix}}(T, \rho_m) + \lambda_w^C(T, \rho_{m,w}) \]
  - critical enhancement for thermal conductivity of water added after mixing

- Calculation of water as hypothetical fluid
  - water could become a liquid under pressure and temperature of moist air
  - treated as hypothetical fluid for \((T<T_c)\) and \((\rho_m > \rho_{m,s})\) as follows
  \[ \eta_w(T, \rho_m) = \eta_w(T, \rho_{m,s}) + \left[ \eta_w(T_{\text{ref}}, \rho_m) - \eta_w(T_{\text{ref}}, \rho_{m,s}) \right] \]
  \[ \lambda_w(T, \rho_m) = \lambda_w(T, \rho_{m,s}) + \left[ \lambda_w(T_{\text{ref}}, \rho_m) - \lambda_w(T_{\text{ref}}, \rho_{m,s}) \right] \]
  with \(T_{\text{ref}} = 650\, \text{K}\) and \(\rho_{m,s}\) as saturated vapor molar density at given temperature

- Quantities for interaction of unlike molecules
  - based on extended corresponding states principle
  - scaling factors resulting for pure components of dry air and water
  with following mixing rules:
  \[ \sigma_{ij} = \frac{1}{2} \left( \sigma_{ii} + \sigma_{jj} \right) \quad \varepsilon_{ij} = \frac{1}{2} \left( \varepsilon_{ii} \varepsilon_{jj} \right)^{1/2} \]
  - \(\sigma_{ij} = 0.31562\, \text{nm}\) and \(\varepsilon_{ij} / k_B = 276.28\, \text{K}\)
  - interaction viscosity in the limit of zero density follows from
  \[ \eta_{ij}^0(T) = \left( \frac{2M_iM_j}{M_i + M_j} \frac{T}{T_{MM}} \right)^{1/2} \]
  \[ \sigma_{ij}^2 S_{\text{MM}}^*(T_{ij}^*) \]
  with \( \ln S_{\text{MM}}^*(T_{ij}^*) = \sum_{k=0}^{4} a_k \left[ \ln(T_{ij}^*) \right]^k \) and \(T_{ij}^* = \frac{k_B T}{\varepsilon_{ij}}\)
  - \(A_{ij}^*\) and \(B_{ij}^*\) are to be 1.1, each
**Improvement of VW Model Using Experimental Data**

- Adjustment of length scaling factor
  - molecules of dry air and water do not correspond to spherically symmetric interaction potentials -> theorem of corresponding states inappropriate for interaction viscosity in the limit of zero density
  - interaction viscosity now treated as function of mole fraction of water
  - fitted to experimental data by Kestin and Whitelaw (1964) as well as by Hochrainer and Munczak (1966) resulting in
    \[
    \sigma_{ij}^{adj}(x_w) = \sigma_{ij} \left[ 1 + x_1x_2 \sum_{k=0}^{n} b_k (x_1 - x_2)^k \right]
    \]
    where coefficients $b_k$ adjusted with $n = 2$

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**Result of Improvement of VW Model Using Experimental Data**

- viscosity of moist air at atmospheric pressure

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3 Kestin and Whitelaw (1964)
4. Results of ASHRAE Research Project RP-1767

4.1 New SI and I-P moist air property tables

New SI and I-P moist air property tables for the ASHRAE Handbook of Fundamentals, Psychrometrics Chapter

<table>
<thead>
<tr>
<th>Temp, °C</th>
<th>Absolute Humidity, kg/kg_dry</th>
<th>Density, kg/m³</th>
<th>Viscosity, μPa s</th>
<th>Kinematic Viscosity, 10⁻⁸ m²/s</th>
<th>Thermal Cond., mW/(m K)</th>
<th>Prandtl Number (α)</th>
<th>Temperature, °C</th>
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<td>1.290</td>
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</table>

Old Figure 12 of the current ASHRAE Handbook of Fundamentals, Psychrometrics Chapter, showing viscosity values for moist air

Regions below red lines are the liquid and ice fog regions.

Mixture model is needed to calculate viscosity in this region!
4.2 New Figures for Transport Properties of Moist Air

New Figure 12 for the ASHRAE Handbook of Fundamentals, Psychrometrics Chapter, showing viscosity values for moist air

Old Figure 13 of the current ASHRAE Handbook of Fundamentals, Psychrometrics Chapter, showing thermal conductivity values for moist air

 Regions below red lines are the liquid and ice fog regions. Mixture model is needed to calculate thermal conductivity in this region!
New Figure 13 for the ASHRAE Handbook of Fundamentals, Psychrometrics Chapter, showing thermal conductivity values for moist air

4.3 Comparison of new algorithms

Comparison of new algorithms for viscosity of moist air to the former equations

<table>
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<tr>
<th>Viscosity</th>
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<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
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<tbody>
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<td>5.59182874</td>
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</tr>
<tr>
<td>Absolute Humidity (converted from Mole Fraction H2O)</td>
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<td>1.86</td>
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<td>1.32</td>
<td>6.64</td>
<td>10.88</td>
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</table>

Tabulated values are calculated as follows: \( \frac{(\text{Moles of Water})}{(\text{Total Mole Fraction})} \times 100 \)

supersaturated moist air
Comparison of new algorithms for thermal conductivity of moist air to the former equations

Relative deviations of the data of Mason and Monchick from the values, calculated from ASHRAE RP-1767, in percent

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Absolute Humidity (converted from Mole Fraction H₂O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<table>
<thead>
<tr>
<th>Mole Fraction H₂O</th>
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<table>
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<th>Relative Deviation</th>
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</table>

supersaturated moist air

4 Mason and Monchick (1965)

4.4 Tables of Transport Properties of Water at Saturation

ASHRAE Handbook Fundamentals, Ch. 1: Table Transport Properties of Water at Saturation (SI Edition)
4.5 Update of Table for Refrigerant 718 (water/steam)

ASHRAE Handbook Fundamentals, Ch. 30: Table Refrigerant 718 (Water/Steam) Properties of Saturated Liquid and Saturated Vapor (SI Edition)

- Saturated water and steam transport properties calculated using latest international IAPWS standards
- State-of-the-art calculation of moist air transport properties consisting of:
  - latest NIST equations for transport properties of dry air
  - current IAPWS formulations for water and steam
  - improvement of the current mixing model for transport properties of moist air
- New SI tables for the ASHRAE Handbook of Fundamentals, Psychrometrics Chapter prepared, I-P tables prepared
- New SI figures 12 and 13 for the ASHRAE Handbook of Fundamentals, Psychrometrics Chapter, I-P figures prepared
- Preparing the Final Report including all equations and coefficients
- Preparing of a research paper for submittal to the Journal Science and Technology for the Built Environment (former HVAC&R Research)

5. Conclusions and Outlook
References


Questions?

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