Property Impacts on Plate-fin Multi-stream Heat Exchanger (Cold Box) Design in CO₂ Cryogenic Process: Part II. Evaluation of Viscosity and Thermal Conductivity Models

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Abstract

Viscosity and thermal conductivity are key transport properties in the design of plate-fin multi-stream heat exchanger in CO₂ cryogenic processes. It is necessary to evaluate the reliabilities of viscosity and thermal conductivity models. In addition, the differences in design of multi-stream heat exchanger by using different property models need to be studied as well. In this paper, viscosity models and thermal conductivity models of CO₂ mixtures with non-condensable gas impurities were evaluated separately by comparison with existing experimental data. Recommendations were given on model selections and their impact on the design of plate-fin multi-stream heat exchanger was analyzed. The results show that for viscosity, the uncertainty range of Wilke’s model is the smallest with a maximum absolute deviation of 6.1%. This model is therefore recommended to be used. For thermal conductivity, GERG model, with a maximum absolute deviation of 8.7% is preferred. The choice of thermal conductivity model has a noticeable impact on the plate-fin multi-stream heat exchanger design, and the maximum deviation by using different thermal conductivity models is 7.5%.

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Keywords: Viscosity, Thermal conductivity, Model evaluation, CO₂ mixture, Multi-stream heat exchanger

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1. Introduction

Part I of the two-paper series has proposed the design procedure for the plate-fin multi-stream heat exchanger and analyzed the property impacts by conducting sensitivity study [1]. It was found that thermal conductivity has the most significant impact while density has the least significant impact. In addition, viscosity was found to have less significant impact than that of heat capacity, but the higher uncertainty range of viscosity models may lead to higher possible deviations in the design of the heat exchanger.

Concerning property model evaluation and recommendations, Li et al. [2-3] assessed and summarized the accuracy of density property models and gave recommendations for density model selection for CO$_2$ mixtures with different impurities at different working conditions. For heat capacity, experimental measurement and model evaluation for CO$_2$ mixtures were also performed [4-6]. For density and heat capacity, different types of models have been compared and analyzed, and recommendations for model selection have also been given. For viscosity and thermal conductivity models, Li et al. [7] collected deviations of different models proposed by different investigators. In addition, some studies have been done regarding modelling, comparison and recommendations for viscosity [8-10] and thermal conductivity [11-14]. However, for viscosity and thermal conductivity, the reliabilities of different models vary for different components and working conditions. Previous studies do not cover all types of models and the wide working conditions for CO$_2$ mixtures with non-condensable gas impurities, and it is still unclear which model(s) should be recommended to use at certain working conditions. Therefore, more work should be done on viscosity and thermal conductivity model evaluation and comparison covering all types of models and a wide range of working conditions. In addition, impacts on the design of multi-stream heat exchangers when different viscosity and thermal conductivity models are used need to be investigated further.

In this paper, as part II of the two-paper series, viscosity models and thermal conductivity models of CO$_2$ mixtures with non-condensable gas impurities were evaluated by comparison to existing experimental data. Recommendations on viscosity and thermal conductivity model selection were given. In addition, the impacts of property model selection on multi-stream heat exchanger design was also analyzed.

2. Property model

2.1. Viscosity models

Three viscosity models and one database, described in Table 1, are used in this study to calculate viscosity of CO$_2$ mixtures.

<table>
<thead>
<tr>
<th>Method</th>
<th>Model</th>
<th>Features</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chapman-Enskog (CE) theory</td>
<td>Wilke</td>
<td>- Collision diameter and collision integrals</td>
<td>[15]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Simplification in kinetic theory approach</td>
<td></td>
</tr>
<tr>
<td>Corresponding state theory</td>
<td>KRW</td>
<td>- With aid of scaling factor</td>
<td>[16] [17]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Empirically determined collision integrals</td>
<td></td>
</tr>
<tr>
<td>Empirical correlation</td>
<td>DS</td>
<td>- Correlated from experimental data</td>
<td>[18]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Appropriate pseudocritical constant rules</td>
<td></td>
</tr>
</tbody>
</table>
2.2. Thermal conductivity model

Five models, described in Table 2, are used in this study to calculate thermal conductivity of CO2 mixtures.

Table 2: Selected models for calculating thermal conductivity of CO2 mixtures

<table>
<thead>
<tr>
<th>Method</th>
<th>Model</th>
<th>Features</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hirschfelder’s equation</td>
<td>WD</td>
<td>Semi-empirical - Standard combining rules</td>
<td>[14]</td>
</tr>
<tr>
<td>Wassiljewa’s equation</td>
<td>KM</td>
<td>Semi-empirical - Reduced rigorous theory</td>
<td>[20]</td>
</tr>
<tr>
<td>Rigorous kinetic theory</td>
<td>MS</td>
<td>Semi-empirical - Simple numerical calculations with few input</td>
<td>[21]</td>
</tr>
<tr>
<td>Empirical correlation</td>
<td>Cheung</td>
<td>Kinetic theory - Energy transport from collisions and diffusion</td>
<td>[22]</td>
</tr>
<tr>
<td>Helmholtz free energy theory</td>
<td>GERG-2004</td>
<td>Fluid-specific correlations and an ECS method - Friction theory method</td>
<td>[19]</td>
</tr>
</tbody>
</table>

3. Collection of experimental data

In order to evaluate the accuracy of the property models, experimental data for viscosity [7, 17, 23-29], and thermal conductivity [11, 14, 20, 30-31] has been collected for CO2 mixtures containing impurities as N2, O2 and Ar. The evaluation was conducted by calculating the deviation between calculated values and experimental data

4. Results and discussion

4.1. Property model evaluation

Table 3 gives the deviations in viscosity values calculated by different viscosity models compared to all experimental data collected in this study. In general, the uncertainty range of Wilke’s model is smallest among all evaluated viscosity models with maximum absolute deviation of -6.1%, while DS has the largest uncertainty range, which is 15.4% in maximum absolute deviation. For KRW and GERG model, the maximum absolute deviation are 10.4% and 6.2% respectively. However, different viscosity models have different performance in predicting viscosity values at different working conditions. For the operating temperature and pressure of cryogenic system (217<T<323 K, 1<P<40 bar), specifically, DS model is recommended to use when temperature is lower than 283 K with maximum deviation of 1.0%. In addition, for temperature higher than 283 K at atmospheric pressure, Wilke model is the first choice to calculate the viscosity of CO2 mixtures with non-condensable impurities with maximum deviation of 4.7%. For pressure higher than atmospheric pressure, GERG model is recommended, the maximum deviations are -3.1%.

Table 3. Evaluation results of viscosity models

<table>
<thead>
<tr>
<th>P (bar)</th>
<th>T (K)</th>
<th>Wilke</th>
<th>KRW</th>
<th>DS</th>
<th>GERG</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>&lt;283</td>
<td>2.9</td>
<td>3.6</td>
<td>1.0</td>
<td>3.3</td>
</tr>
<tr>
<td>1</td>
<td>&gt;283</td>
<td>4.7</td>
<td>5.6</td>
<td>-5.0</td>
<td>6.2</td>
</tr>
<tr>
<td>1-20</td>
<td>293</td>
<td>-2.5</td>
<td>-1.0</td>
<td>-6.7</td>
<td>-0.4</td>
</tr>
<tr>
<td>20-60</td>
<td>289</td>
<td>-6.1</td>
<td>10.4</td>
<td>-15.4</td>
<td>-3.1</td>
</tr>
<tr>
<td>Overall</td>
<td></td>
<td>-6.1/4.7</td>
<td>-1.2/10.4</td>
<td>-15.4/3.8</td>
<td>-1.0/6.2</td>
</tr>
</tbody>
</table>

Table 4 gives the deviations in thermal conductivity values calculated by different models compared to all experimental data. According to the statistic, the uncertainty range of GERG model is smallest among all evaluated thermal conductivity models with maximum absolute deviation of 8.7%, therefore GERG model is recommended for predicting thermal conductivity values of CO2 mixtures with non-condensable...
gas impurities. WD has the largest uncertainty range, which is 16.7% in maximum absolute deviation. Cheung model is the best second to GERG model, the uncertainty range is within 9.6%. In addition, KM and MS model have the uncertainty range of 12.6% and 13.2% respectively. However, different thermal conductivity models have different performance in predicting thermal conductivity values at different working conditions. For the operating temperature and pressure of cryogenic system (217<T<323 K, 1<P<40 bar), specifically, GERG is recommended for temperatures higher than 273 K at atmospheric pressure for which the maximum deviation is 8.7%. For pressures higher than atmospheric pressure, the KM model is preferred at pressures lower than 30 bar, and GERG should be employed when the pressure is higher than 30 bar. For temperature lower than 273 K, there is no experimental data for evaluation, therefore it is still not known which model is more accurate.

Table 4. Evaluation results of thermal conductivity models

<table>
<thead>
<tr>
<th>P (bar)</th>
<th>T (K)</th>
<th>Maximum Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>&gt;273</td>
<td>16.7</td>
</tr>
<tr>
<td>1-30</td>
<td>296</td>
<td>5.2</td>
</tr>
<tr>
<td>&gt;30</td>
<td>380</td>
<td>13.1</td>
</tr>
<tr>
<td>Overall</td>
<td></td>
<td>-9.6/16.7</td>
</tr>
</tbody>
</table>

4.2. Impacts of property model selection on heat exchanger design

Fig. 1 presents the design volume of the heat exchanger using different viscosity models including GERG, Wilke, KRW and DS. Wilke model is recommended to use according to the results of model evaluation. As shown in the Fig. 1, the overall volume of the heat exchanger is 23.4 m³, 23.3 m³, 23.3 m³ and 23.1 m³ when using GERG, Wilke, KRW and DS respectively, and the deviations in volumes are 0.5% (GERG), -0.3% (KRW) and -0.9% (DS) respectively comparing to the volume when using the Wilke model. Thus the selection of viscosity model has little impact on the calculation of the plate-fin multi-stream heat exchanger volume in CO₂ cryogenic processes.

Fig. 1 (a) Design volume of heat exchanger by using different viscosity models; (b) Design volume of heat exchanger by using different thermal conductivity models

Fig. 2 illustrates the design volume of the heat exchanger using different thermal conductivity models including GERG, WD, KM, MS and Cheung. The GERG model is recommended to be use according to the results of the model evaluation. As shown in the Fig.2, the overall volume of the heat exchanger is 23.4 m³, 22.4 m³, 22.9 m³, 24.2 m³ and 23.0 m³ by using GERG, WD, KM, MS and Cheung respectively, and the deviations in volumes are -4.2% (WD), 2.0% (KM), 3.4% (MS) and -1.6% (Cheung) respectively comparing to the volume when using the GERG model. In addition, the maximum deviation of the heat
exchanger volume using different models is 7.5%, occurring when WD and MS are compared. Thus the selection of thermal conductivity model has a noticeable impact on the calculated volume of the plate-fin multi-stream heat exchanger in CO₂ cryogenic processes.

5. Conclusion:
In this study, viscosity models (including GERG, Wilke, KRW, and DS) and thermal conductivity models (including GERG, WD, KM, MS, and Cheung) of CO₂ mixtures with non-condensable impurities were evaluated by comparison with existing experimental data. Recommendation of viscosity and thermal conductivity model selection was given. In addition, impacts of property model selection on heat exchanger design were analyzed. The following conclusions can be drawn:
- For viscosity, Wilke’s model shows the smallest uncertainty range with a maximum absolute deviation of 6.1%, and is therefore recommended to be used. The DS model is recommended when temperatures are lower than 283 K. For temperatures higher than 283 K at atmospheric pressure, the Wilke model is the first choice. For pressures higher than atmospheric pressure, the GERG model is recommended.
- For thermal conductivity, the uncertainty range of GERG model is the smallest among all evaluated thermal conductivity models with a maximum absolute deviation of 8.7%, and therefore the GERG model is recommended. For specific conditions, GERG is recommended for temperatures higher than 273 K at atmospheric pressure. For pressures higher than atmospheric pressure, KM model is preferred at pressures lower than 30 bar, and GERG should be employed when the pressure is higher than 30 bar.
- The choice of thermal conductivity model has a noticeable impact on the plate-fin multi-stream heat exchanger design, while the choice of viscosity model has little impact. The maximum deviation by using different thermal conductivity models is 7.5%.

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References


**Biography**

Yuting Tan now is a Ph.D. student in Royal Institute of Technology (KTH) working on carbon capture and storage (CCS).