Carbon Dioxide Capture and Acid Gas Injection
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Edited by

Ying Wu, John J. Carroll and Weiyao Zhu
# Contents

<table>
<thead>
<tr>
<th>Preface</th>
<th>xiii</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1</strong> Enthalpies of Carbon Dioxide-Methane and Carbon Dioxide-Nitrogen Mixtures: Comparison with Thermodynamic Models</td>
<td>1</td>
</tr>
<tr>
<td><em>Erin L. Roberts and John J. Carroll</em></td>
<td></td>
</tr>
<tr>
<td>1.1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Enthalpy</td>
<td>2</td>
</tr>
<tr>
<td>1.3 Literature Review</td>
<td>2</td>
</tr>
<tr>
<td>1.3.1 Carbon Dioxide-Methane</td>
<td>4</td>
</tr>
<tr>
<td>1.3.2 Carbon Dioxide-Nitrogen</td>
<td>4</td>
</tr>
<tr>
<td>1.4 Calculations</td>
<td>5</td>
</tr>
<tr>
<td>1.4.1 Benedict-Webb-Rubin</td>
<td>6</td>
</tr>
<tr>
<td>1.4.2 Lee-Kesler</td>
<td>12</td>
</tr>
<tr>
<td>1.4.3 Soave-Redlich-Kwong</td>
<td>17</td>
</tr>
<tr>
<td>1.4.4 Peng-Robinson</td>
<td>23</td>
</tr>
<tr>
<td>1.4.5 AQUAlicibrium</td>
<td>28</td>
</tr>
<tr>
<td>1.5 Discussion</td>
<td>33</td>
</tr>
<tr>
<td>1.6 Conclusion</td>
<td>36</td>
</tr>
<tr>
<td>References</td>
<td>37</td>
</tr>
</tbody>
</table>

**2** Enthalpies of Hydrogen Sulfide-Methane Mixture: Comparison with Thermodynamic Models | 39 |
| *Erin L. Roberts and John J. Carroll* | |
| 2.1 Introduction | 39 |
| 2.2 Enthalpy | 40 |
| 2.3 Literature Review | 40 |
| 2.4 Calculations | 41 |
| 2.4.1 Lee-Kesler | 41 |
| 2.4.2 Benedict-Webb-Rubin | 43 |
| 2.4.3 Soave-Redlich-Kwong | 43 |
3 Phase Behavior and Reaction Thermodynamics Involving Dense-Phase CO₂ Impurities 55
   J.A. Commodore, C.E. Deering and R.A. Marriott
   3.1 Introduction 55
   3.2 Experimental 57
   3.3 Results and Discussion 58
      3.3.1 Phase Behavior Studies of SO₂ Dissolved in Dense CO₂ Fluid 58
      3.3.2 The Densimetric Properties of CS₂ and CO₂ Mixtures 60
   References 61

4 Sulfur Recovery in High Density CO₂ Fluid 63
   S. Lee and R.A. Marriott
   4.1 Introduction 64
   4.2 Literature Review 64
   4.3 Methodology 65
   4.4 Results and Discussion 66
   4.5 Conclusion and Future Directions 67
   References 68

5 Carbon Capture Performance of Seven Novel Immidazolium and Pyridinium Based Ionic Liquids 71
   Mohamed Zoubeik, Mohanned Mohamedali and Amr Henni
   5.1 Introduction 71
   5.2 Experimental Work 73
      5.2.1 Materials 73
      5.2.2 Density Measurement 73
      5.2.3 Solubility Measurement 73
   5.3 Modeling 76
      5.3.1 Calculation of Henry’s Law Constants 76
      5.3.2 Critical Properties Calculations 76
      5.3.3 Peng Robinson EoS 76
5.4 Results and Discussion 77
  5.4.1 Density 77
  5.4.2 Critical Properties 77
  5.4.3 CO$_2$ Solubility 78
  5.4.4 The Effect of Changing the Cation 81
  5.4.5 The Effect of Changing the Anion 84
  5.4.6 Henry's Law Constant, Enthalpy and Entropy Calculations 85
  5.4.7 Thermodynamic Modeling of CO$_2$ Solubility 86

5.5 Conclusion 87
Acknowledgements 88
References 88

6 Vitrisol® a 100% Selective Process for H$_2$S Removal in the Presence of CO$_2$ 91

W.N. Wermink, N. Ramachandran, and G.F. Versteeg

6.1 Introduction 92
6.2 Case Definition 94
6.3 "Amine-Treated" Cases by PPS 95
  6.3.1 Introduction to PPS 95
  6.3.2 Process Description 96
  6.3.3 PFD 97
  6.3.4 Results 97
    6.3.4.1 Case 1 97
    6.3.4.2 Case 2 97

6.4 Vitrisol® Process Extended with Regeneration of Active Component 99
  6.4.1 Technology Description 99
  6.4.2 Parameters Determining the Process Boundary Conditions 99
  6.4.3 Absorption Section 101
  6.4.4 Regeneration Section 102
  6.4.5 Sulphur Recovery Section 104
  6.4.6 CO$_2$-Absorber 105
  6.4.7 PFD 105

6.5 Results 105
6.6 Discussion 110
  6.6.1 Comparison of Amine Treating Solutions to Vitrisol® 110
  6.6.2 Enhanced H$_2$S Removal of Barnett Shale Gas (case 2) 112
6.7 Conclusions 113
6.8 Notation 115
References 115
Appendix 6-A: H&M Balance of Case 1 (British Columbia shale) of the Amine Process 117
Appendix 6-B H&M Balance of Case 2a (Barnett shale) of the Amine Process with Stripper Promoter 119
Appendix 6-C H&M Balance of Case 3 (Barnett shale) of the Amine Process (MEA) 121
Appendix 6-D: H&M Balance of Case 1 (British Columbia shale) of the Vitrisol® process 123
Appendix 6-E H&M Balance of Case 2 (Barnett shale) of the Vitrisol® Process 125

7 New Amine Based Solvents for Acid Gas Removal 127
Yohann Coulier, Elise El Ahmar, Jean-Yves Coxam, Elise Provost, Didier Dalmazzone, Patrice Paricaud, Christophe Coquelet and Karine Ballerat-Busserolles
7.1 Introduction 128
7.2 Chemicals and Materials 131
7.3 Liquid-Liquid Equilibria 131
  7.3.1 LLE in {methylpiperidines – H$_2$O} and {methylpiperidines – H$_2$O – CO$_2$} 131
  7.3.2 Liquid-Liquid Equilibria of Ternary Systems {Amine – H$_2$O – Glycol} 135
  7.3.3 Liquid-Liquid Equilibria of the Quaternary Systems {CO$_2$ – NMPD – TEG – H$_2$O} 136
7.4 Densities and Heat Capacities of Ternary Systems {NMPD – H$_2$O – Glycol} 137
  7.4.1 Densities 137
  7.4.2 Specific Heat Capacities 137
7.5 Vapor-Liquid Equilibria of Ternary Systems {NMPD – TEG – H$_2$O – CO$_2$} 139
7.6 Enthalpies of Solution 140
7.7 Discussion and Conclusion 143
Acknowledgments 143
References 144
8 Improved Solvents for CO₂ Capture by Molecular Simulation Methodology
William R. Smith
8.1 Introduction 147
8.2 Physical and Chemical Models 149
8.3 Molecular-Level Models and Algorithms for Thermodynamic Property Predictions 150
8.4 Molecular-Level Models and Methodology for MEA–H₂O–CO₂ 153
8.4.1 Extensions to Other Alkanolamine Solvents and Their Mixtures 155
Acknowledgements 157
References 157

9 Strategies for Minimizing Hydrocarbon Contamination in Amine Acid Gas for Reinjection
Mike Sheilan, Ben Spooner and David Engel
9.1 Introduction 162
9.2 Amine Sweetening Process 162
9.3 Hydrocarbons in Amine 164
9.4 Effect of Hydrocarbons on the Acid Gas Reinjection System 166
9.5 Effect of Hydrocarbons on the Amine Plant 167
9.6 Minimizing Hydrocarbon Content in Amine Acid Gas 171
9.6.1 Option 1. Optimization of the Amine Plant Operation 171
9.6.2 Option 2. Amine Flash Tanks 176
9.6.3 Option 3. Rich Amine Liquid Coalescers 178
9.6.4 Option 4. Use of Skimming Devices 180
9.6.5 Option 5. Technological Solutions 182
References 183

10 Modeling of Transient Pressure Response for CO₂ Flooding Process by Incorporating Convection and Diffusion Driven Mass Transfer
Jianli Li and Gang Zhao
10.1 Introduction 186
10.2 Model Development 187
10.2.1 Pressure Diffusion 187
10.2.2 Mass Transfer 188
10.2.3 Solutions 190
10.3 Results and Discussion 191
10.3.1 Flow Regimes 191
10.3.2 Effect of Mass Transfer 192
10.3.3 Sensitivity Analysis 195
10.3.3.1 CO$_2$ Bank 195
10.3.3.2 Reservoir Outer Boundary 196
10.4 Conclusions 196
Acknowledgments 197
References 197

11 Well Modeling Aspects of CO$_2$ Sequestration 199

Liaqat Ali and Russell E. Bentley
11.1 Introduction 199
11.2 Delivery Conditions 200
11.3 Reservoir and Completion Data 201
11.4 Inflow Performance Relationship (IPR) and Injectivity Index 201
11.5 Equation of State (EOS) 202
11.6 Vertical Flow Performance (VFP) Curves 205
11.7 Impact of the Well Deviation on CO$_2$ Injection 208
11.8 Implication of Bottom Hole Temperature (BHT) on Reservoir 209
11.9 Impact of CO$_2$ Phase Change 213
11.10 Injection Rates, Facility Design Constraints and Number of Wells Required 214
11.11 Wellhead Temperature Effect on VFP Curves 214
11.12 Effect of Impurities in CO$_2$ on VFP Curves 216
11.13 Concluding Remarks 217
Conversion Factors 218
References 218


Qi Li, Xiaying Li, Zhiyong Niu, Dongqin Kuang, Jianli Ma, Xuehao Liu, Yankun Sun and Xiaochun Li
12.1 Introduction 222
12.2 The Amu Darya Right Bank Gas Reservoirs in Turkmenistan 223
12.3 Model Development 223
  12.3.1 State equation 224
    12.3.1.1 Introduction of Traditional PR State Equation 224
    12.3.1.2 Modifications for the Vapor-Aqueous System 224
  12.3.2 Salinity 225
  12.3.3 Diffusion 226
    12.3.3.1 Diffusion Coefficients 226
    12.3.3.2 The Cross-Phase Diffusion Coefficients 226

12.4 Simulation Model 227
  12.4.1 Model Parameters 227
  12.4.2 Grid-Sensitive Research of the Model 227
  12.4.3 The Development and Exploitation Mode 230

12.5 Results and Discussion 230
  12.5.1 Reservoir Pressure 230
  12.5.2 Gas Sequestration 232
  12.5.3 Production 235
  12.5.4 Recovery Ratio and Recovery Percentage 238

12.6 Conclusions 239

12.7 Acknowledgments 240

References 241

Index 245
Preface

The Sixth International Acid Gas Injection Symposium (AGIS VI) was held in Houston, Texas, in September 2016. As with previous Symposia, the focus of AGIS VI was the injection of acid gas (CO₂, H₂S, and mixtures of these components) for the purposes of disposal or for enhanced oil and/or gas recovery. This book contains select papers from the Symposium in Houston.

The capture of carbon dioxide from flue gas and its disposal into a subsurface geological formation remains a viable option for the clean use of hydrocarbon fuels. The related technology is acid gas injection. Here the H₂S and CO₂ are removed from raw natural gas. This volume contains papers directly related to these two topics ranging from the physical properties of the gas mixtures, evaluation of new and existing solvents, and subsurface engineering aspects of the process. Furthermore, contributors came from Canada, Europe, and China, as well as from the host country, the United States. And this is reflected in the papers in this volume.

On a very sad note, Marco Satyro passed away on September 8, 2016, just prior to the Symposium. Marco was a good friend of AGIS being an active member of the Technical Committee for many years. He contributed many papers and encouraged many others to participate. At the first AGIS he presented the paper “The Performance of State of the Art Industrial Thermodynamic Models for the Correlation and Prediction of Acid Gas Solubility in Water” and this paper appeared in the first volume of the Advances in Natural Gas Engineering. He also was the coauthor of several other contributions to the Series and they are listed below. This volume is dedicated to the memory of Dr. Satyro.

References – papers of M.A. Satyro from the Advances in Natural Gas Engineering series.


1

Enthalpies of Carbon Dioxide-Methane and Carbon Dioxide-Nitrogen Mixtures: Comparison with Thermodynamic Models

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Abstract

The physical properties of acid-gas injection streams are important for use in design considerations of the acid-gas scheme. One such property is the enthalpy of the stream. As carbon dioxide is rarely pure, with methane and nitrogen being common impurities in the stream, the effect of these impurities on the enthalpy is also important to consider.

This study compares experimentally determined excess enthalpies and enthalpy departures from literature to the enthalpy predictions of five different models, Benedict-Webb-Rubin, Lee-Kesler, Soave-Redlich-Kwong, and Peng-Robinson from VMGSim, as well as AQUAlibrium software. The mixtures studied are carbon dioxide-methane, as well as carbon dioxide- nitrogen mixtures at a wide range of compositions.

The Soave-Redlich-Kwong model gave the most accurate predictions for both the excess enthalpies and enthalpy departures, with Lee-Kesler frequently giving the least accurate predictions for the mixtures.

1.1 Introduction

An increase in demand of natural gas has led producers to pursue poorer quality reservoirs. These contain higher levels of carbon dioxide that then must be responsibly disposed. Regulations prevent the flaring of the acid-gas mixtures, therefore requiring an alternate means of disposal. One such method is the injection of acid gas into subsurface reservoirs.
An understanding of the physical properties of the stream is essential in the design of the acid-gas injection scheme. The enthalpy of the stream is required in the design of the compressor for injection. Common impurities in the carbon dioxide include methane and nitrogen; therefore the effect of these impurities on the enthalpy of carbon dioxide is required for design.

This paper investigates the accuracy of five different thermodynamic models for predicting such mixtures. Four different equations of state, Benedict-Webb-Rubin (BWR), Lee-Kesler (LK), Soave-Redlich-Kwong (SRK), Peng-Robinson (1978) were used with VMGSim software, as well as the AQUAlibrium model. BWR and LK are multi-constant equations, and SRK and PR78 are cubic equations of state. The AQUAlibrium model uses a variation of Peng-Robinson.

1.2 Enthalpy

The enthalpy of mixtures can be determined in a number of ways. One method is to use excess enthalpy (enthalpy of mixing). Excess enthalpy is defined as

\[ H^E = \left[ H_m - \sum_i x_i H_i \right] \] (1.1)

where:  
\[ H^E \] – Excess enthalpy  
\[ H_m \] – Enthalpy of mixture  
\[ H_i \] – Enthalpy of component \( i \)  
\[ x_i \] – mol fraction of component \( i \)

Alternatively, the enthalpy of the mixture can be represented as an enthalpy departure, a difference between the enthalpy at a given pressure, and the enthalpy at a reference pressure while keeping the temperature constant.

Enthalpies can be expressed in J/mol, or for greater relevance to acid-gas injection design, can be expressed in HP/MMSCFD. The conversion between units is 1 HP/MMSCFD to 53.86 J/mol.

1.3 Literature Review

A review of literature was performed to compile experimental data for the enthalpy of carbon dioxide-methane mixtures as well as carbon dioxide-nitrogen mixtures. Table 1.1 summarizes the relevant data used in this study.
Table 1.1 Summary of experimental data of enthalpy of carbon dioxide mixtures.

<table>
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<tr>
<th>Temperature (°C)</th>
<th>Pressure (MPa)</th>
<th>Composition (mol% CO₂)</th>
<th>Impurity</th>
<th>Comments</th>
<th>Ref.</th>
</tr>
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| 10–80            | 1–11           | 0.1–0.9                | Methane  | • Excess enthalpies  
                  |                 |           |          | • All vapour enthalpies  
                  |                 |           |          | • 646 data points       | 1    |
| 20, 32, 40       | 0.5–4.6        | 0.1–0.9                | Methane  | • Excess enthalpies  
                  |                 |           |          | • All vapour enthalpies  
                  |                 |           |          | • 60 data points        | 2    |
| 0–90             | 3–13.7         | 0.145, 0.423           | Methane  | • Enthalpy departure  
                  |                 |           |          | • Liquid and vapour densities  
                  |                 |           |          | • 42 data points        | 3    |
| –46–149          | 0.7–13.8       | 0.5                    | Methane  | • Enthalpy departure  
                  |                 |           |          | • Liquid and vapour densities  
                  |                 |           |          | • 46 data points        | 4    |
| 40               | 1–12           | 0.1–0.9                | Nitrogen | • Excess enthalpies  
                  |                 |           |          | • All vapour enthalpies  
                  |                 |           |          | • 108 data points       | 5    |
| 31, 40           | 3.5, 6.5       | 0.2–0.7                | Nitrogen | • Excess enthalpies  
                  |                 |           |          | • All vapour enthalpies  
                  |                 |           |          | • 27 data points        | 6    |

1. Lee & Mather (1972)  
2. Barry et al. (1982)  
3. Ng & Mather (1976)  
6. Hejmadi et al. (1971)
1.3.1 Carbon Dioxide-Methane

The most extensive study performed for enthalpies of carbon dioxide-methane mixtures was performed by Lee & Mather (1972). Their study consisted of mol fractions of 0.1–0.9, taken at intervals of 0.1, for a total of 9 different mol fractions. Measurements of excess enthalpy were reported at 8 different temperatures from 10–80 °C, with ranges of pressure of 1.0–4.4 MPa for 10 °C, 1.0–5.07 for 20 °C, 1.0–11.1 for 40 °C, and 1.0–10.1 for 32 °C, 50 °C, 60 °C, 70 °C, and 80 °C. In total, 648 data points were reported. Two typographical errors were found in the data set; they are not included in the numerical error analysis but are represented in the figures.

Another smaller study was performed by Barry et al. (1982), for excess enthalpies of carbon dioxide-methane mixtures. Data was taken at three different temperatures, 20 °C, 32 °C, and 40 °C. Seven different pressures were used, ranging from 0.51 MPa to 4.6 MPa, with pressure of over 2 MPa only being measured for 40 °C. The mol fractions measured were not taken in increments, instead were taken at a wide variety of fractions ranging from 0.1 to 0.9.

Two other studies were done using enthalpy departures by Ng & Mather (1976) and Peterson & Wilson (1974). Ng & Mather (1976) used pressures of 3–13.7 MPa, and temperatures of 0–90 °C for mol fractions of 0.145 and 0.423. They used the ideal gas enthalpy as a reference point to measure the enthalpy departure. Peterson & Wilson (1974) only measured equimolar mixtures of carbon dioxide and methane with pressures from 0.7–13.8 MPa and temperatures of 255.4 K–422 K. The reference enthalpy used was measured at a pressure of 0.138 MPa. These two studies were the only ones that measured both liquid and vapor enthalpies, instead of just vapor.

1.3.2 Carbon Dioxide-Nitrogen

Lee & Mather (1970) and Hejmadi et al. (1971) studied the excess enthalpies of carbon dioxide-nitrogen mixtures. Lee & Mather (1970) looked at mole fractions from 0.1–0.9 at intervals of 0.1. Pressures from 1.01 MPa to 12.16 MPa were used, at only a single temperature of 40 °C.

Hejmadi et al. (1971) used only two different temperatures of 31 °C and 40 °C, and two different pressures of 3.5 MPa and 6.5 MPa. They used mole fraction of nitrogen from 0.2–0.7.
1.4 Calculations

The experimental enthalpies were compared to calculated enthalpies using BWR, LK, SRK, and PR78 thermodynamic models from VMGSim software, as well as using AQUAlibrium software.

The six different mixtures (four with methane, two with nitrogen) as summarized in Table 1.1 were evaluated. Four error functions for both the excess enthalpies and the enthalpy departures were used to analyze the accuracy of the prediction of each method.

For the excess enthalpies, the absolute average difference (AAD) was defined as:

$$\text{AAD} = \frac{1}{NP} \sum \left| H_{\text{exp}}^E - H_{\text{calc}}^E \right|$$

(1.2)

where:  
NP – number of points  
$H_{\text{exp}}^E$ – experimental excess enthalpy  
$H_{\text{calc}}^E$ – calculated excess enthalpy

and the average difference (AD) was defined as:

$$\text{AD} = \frac{1}{NP} \sum \left( H_{\text{exp}}^E - H_{\text{calc}}^E \right)$$

(1.3)

The absolute average error (AAE) in excess enthalpies was defined as:

$$\text{AAE} = \frac{1}{NP} \sum \left| \frac{H_{\text{exp}}^E - H_{\text{calc}}^E}{H_{\text{calc}}^E} \right| \times 100\%$$

(1.4)

and the average error (AE) was defined as:

$$\text{AE} = \frac{1}{NP} \sum \frac{H_{\text{exp}}^E - H_{\text{calc}}^E}{H_{\text{calc}}^E} \times 100\%$$

(1.5)

For enthalpy departures, the absolute average difference

$$\text{AAD} = \frac{1}{NP} \sum \left| (H^o - H)_{\text{exp}} - (H^o - H)_{\text{calc}} \right|$$

(1.6)
where \( H^o \) – enthalpy of mixture at reference pressure
\( H \) – enthalpy of mixture at measured pressure
and the average difference was defined as:

\[
AD = \frac{1}{NP} \sum (H^o - H)_{exp} - (H^o - H)_{calc}
\] (1.7)

The absolute average error for enthalpy departure was defined as:

\[
AAE = \frac{1}{NP} \sum \left| \frac{(H^o - H)_{exp} - (H^o - H)_{calc}}{(H^o - H)_{calc}} \right| \times 100\% \] (1.8)

and the average error was defined as:

\[
AE = \frac{1}{NP} \sum \frac{(H^o - H)_{exp} - (H^o - H)_{calc}}{(H^o - H)_{calc}} \times 100\% \] (1.9)

### 1.4.1 Benedict-Webb-Rubin

For the Lee & Mather (1972) methane data of excess enthalpies, the AAD was 78.1 J/mol and the AD was 2.6 J/mol. The AAE was 19.0% and the AE was -14.6%. The maximum difference was 2113.2 J/mol occurring at 8.11 MPa and a mole fraction of 0.2. The maximum error was 131.7% at the same conditions as the maximum difference. At lower pressures, the enthalpies were overestimated, and at the higher pressures they were underestimated. The greatest deviations occurred when there was a rapid change in enthalpy with pressure. This occurred at around 7–10 MPa for the 32 °C and 40 °C temperatures. There was also a very large difference between the calculated and experimental enthalpy for the 10.13 MPa isobar at 50 °C. Figures 1.1 through 1.8 show the experimental and calculated enthalpies for the different temperatures.

The Barry et al. (1982) methane data of excess enthalpies had an AAD of 9.1 J/mol, an AD of -8.3 J/mol, an AAE of 14.2% and an AE of -11.0%. The maximum difference was 46.5 J/mol at 4.6 MPa, 40 °C and 0.351 mole fraction methane. The maximum error was 42.5% at 0.53 MPa, 32 °C and 0.63 mole fraction methane. The deviations are smaller due to the lower pressure range of the data.

The Lee & Mather (1970) nitrogen data of excess enthalpies taken at 40 °C had similar results as the Lee & Mather (1972) methane data for the 40 °C data, with the greatest difference occurring at 9.12 MPa. The
Figure 1.1 Experimental and calculated enthalpies at 10 °C using BWR (Lee & Mather, 1972).

Figure 1.2 Experimental and calculated enthalpies at 20 °C using BWR (Lee & Mather, 1972).
Figure 1.3 Experimental and calculated enthalpies at 32 °C using BWR (Lee & Mather, 1972).

Figure 1.4 Experimental and calculated enthalpies at 40 °C using BWR (Lee & Mather, 1972).
Figure 1.5 Experimental and calculated enthalpies at 50 °C using BWR (Lee & Mather, 1972).

Figure 1.6 Experimental and calculated enthalpies at 60 °C using BWR (Lee & Mather, 1972).
**Figure 1.7** Experimental and calculated enthalpies at 70 °C using BWR (Lee & Mather, 1972).

**Figure 1.8** Experimental and calculated enthalpies at 80 °C using BWR (Lee & Mather, 1972).
AAD was 151.1 J/mol, the AD was 58.7 J/mol, the AAE was 15.0% and the AE was –0.7%. The maximum difference was 969.8 J/mol at 9.1 MPa, and 0.1 mole fraction nitrogen. The maximum error was 70% at the same conditions as the maximum difference. Figure 1.9 shows the calculated and experimental enthalpies for the BWR model at 40 °C.

The Hejmadi et al. (1971) nitrogen of excess enthalpies data had an AAD of 26.1 J/mol, and AD of –11.0 J/mol, an AAE of 9.5% and an AE of –7.9%. The maximum difference was 90.8 J/mol at 6.5 MPa, 31 °C, and 0.239 mole fraction nitrogen. The maximum error was 14.1% at 3.4 MPa, 40 °C and 0.67 mole fraction nitrogen. As with the Barry et al. (1982) methane data, the lower deviations are likely due to the lower pressure range used in the measurements, as the highest pressure used was 6.5 MPa and the greatest deviations typically occurred around 7–10 MPa for temperatures in the 30–40 °C range.

For the Peterson & Wilson (1974) methane data for enthalpy departures, the AAD was 56.4 J/mol, the AD was 26.2 J/mol, the AAE was 3.7% and the AE was 1.4%. Two points were omitted from the error calculations.