CHAPTER 5

Experimental Procedure

5.1 Experimental Procedure

Five palladium test beds are employed in this experiment shown in Figure 5.1. Each of the test beds is loaded to a different pressure, for example, in the first data set, shown in Appendix A, the test beds were loaded at 20°C, to 667, 2502, 4022, 6340, and 10303 psia. The temperature of the environmental chamber was set to 20°C, and the test beds were allowed to equilibrate to this temperature.

Figure 5.1 Five Beds Utilized in the Experiment.

Five different test beds are being utilized in this experiment, shown in Figure 5.1. The five beds will be achieve equilibrium at 20°C. Approximately 50 psia of hydrogen is
in the high-pressure manifold. The environmental chamber will be opened and the five beds will be opened with a half turn of the AE 30,000 psia valves. This is the beginning of the loading of the beds.

A calculation of the predicted pressures is done using the Fortran program Fill2, shown in the Appendix B, (Meyer, 1996). The inputs for the program are the moles of hydrogen, the amount of palladium in grams, the free volume of the un-hydrided unit, and the ambient temperature. The program can predict the pressure and the fugacity of the bed at different temperatures. When the maximum pressure at the highest temperature is needed a calculation of the initial loading pressure at 20°C is calculated.

5.2 Pressure Loading of the Beds

The initial loading of the each of the beds is at a different pressure. All of the beds are then controlled to an equilibrium baseline temperature of 20°C. The temperature and pressure are monitored every 15 minutes until equilibrium is reached. With this experimental setup the beds reach equilibrium in approximately 1 hour, the actual time for equilibration is shown in Appendix A. The baseline temperature, outside temperature of the outside valve and pressure are taken for each of the beds after equilibrium is reached. The temperature of the environmental chamber is then changed to another temperature and the process is repeated. In the first three P-C-T experiments the temperature of the baseline was 20°C. Then the beds were cycled through the temperatures 0°C, -20°C, -40°C, -60°C, 20°C, 40°C, 60°C, 80°C, 100°C, 120°C, 20°C and 20°C. Between the last two 20°C temperatures the chamber door is opened and the valve directly next to the palladium test beds is closed. When this valve is closed the
pressures within this now closed system change because of the movement of the valve seat slightly changes the internal volume. This volume change is on the order of \( \approx 0.05 \) to 0.1 \( \text{cm}^3 \). At the 10,000 psia this change in volume increases the pressure by 35 psia. It is important to note that closing the valve will change the pressure in the palladium test bed.

### 5.3 Bed Weighing Procedure

When the test beds equilibrate at the last temperature the valves directly next to the beds are closed. When closed the last pressure and temperature data points are taken. Each of the beds is then individually disconnected from the high-pressure manifold, shown in Figure 5.2.

![Diagram Showing Disconnection of Test Bed](image)

**Figure 5.2. Diagram Showing Disconnection of Test Bed.**

The beds are weighed to determine the amount of hydrogen within the bed. When handling a test beds, latex gloves are worn to minimize the possibility of adding contaminants to the beds. When measuring the weights one person is weighing the beds and another person is writing the weight down and verifying the correct weights are taken. The mass balance is first calibrated using a 2000.000gm weight. After the calibration the 2000gm standard weight is measured 3 times to insure that the balance is reading correctly. The standard weight must be repeatable to \( \pm 0.002 \) gm. The bed is then
Figure 5.3 Bed Placement on the Balance Pan.
placed on the balance with special consideration to place the center of gravity of the bed in the center of the balance pan. The placement of a test bed is shown in a photograph in Figure 5.3.

The bed weight is then taken three times to insure that the test bed weight is within the 0.001 gm tolerance. After the three weights are taken the standard weight is then placed on the balance and weighed. The 2000gm standard weight traceable to NIST is weighed and must be within the ±0.002gm of the initial weight. Each bed is weighed using this procedure.
CHAPTER 6

Results and Discussion

6.1 Calculation of the Fugacity and Compressibility Factor

The fugacity-composition-temperature curves describe the equation of state for the palladium hydrogen system. The fugacity is calculated from the following integral equations:

\[
\ln\left(\frac{f}{P'}\right) = \int_0^{P'} \frac{Z - 1}{P} \, dP
\]  

(6-1)

where the compressibility factor, \(Z\) is defined by

\[
Z = \frac{Pv}{RT}
\]  

(6-2)

It is more convenient to write fugacity in terms of fugacity coefficient, \(\Phi\) as:

\[
\ln \Phi = \int_0^{P_{\text{tot}}} (Z - 1) \, d\ln P
\]  

(6-3)

where

\[f = \Phi P\]  

(6-4)

The fugacity coefficient with a conversion to atmospheres becomes:

\[
\Phi = e^{((C_0 + C_1 T + C_2 T^2)(\frac{P}{T}) + (C_3 + C_4 T + C_5 T^2)\frac{1}{2}(\frac{P}{T})^2 + (C_6 + C_7 T + C_8 T^2)\frac{1}{3}(\frac{P}{T})^3 + (C_9 + C_1 T + C_{11} T^2)\frac{1}{4}(\frac{P}{T})^4)}
\]  

(6-5)

Where \(C_0, C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{11}\) are compressibility constants for the compressibility factor \(Z\), pressure \(P\) is in atmospheres. The compressibility factor \(Z\) is in the form of the equation:
\[ Z = 1 + (C_0 + C_1 T + C_3 T^2)(\frac{P}{T}) + (C_4 + C_5 T + C_6 T^2)(\frac{P}{T})^2 \\
+ (C_7 + C_8 T + C_9 T^2)(\frac{P}{T})^3 + (C_{10} + C_{11} T + C_{12} T^2)(\frac{P}{T})^4 \]  

(6-6)

The compressibility constants used in equations (6-5) and (6-6) are in Table 6.1, from (Meyer, 1996).

<table>
<thead>
<tr>
<th>(C_1)</th>
<th>(C_2)</th>
<th>(C_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.022456</td>
<td>8.3057e-4</td>
<td>-1.0193e-6</td>
</tr>
<tr>
<td>-1.9111e-4</td>
<td>1.5657e-7</td>
<td></td>
</tr>
<tr>
<td>-8.1655e-6</td>
<td>3.0139e-8</td>
<td></td>
</tr>
<tr>
<td>-1.5121e-4</td>
<td>2.7545e-6</td>
<td>-4.6721e-9</td>
</tr>
</tbody>
</table>

### 6.2 Calculation of the Atomic Ratio

The moles of hydrogen within the palladium lattice (palladium solid) are calculated. The weight of the hydrogen measured on the mass balance is the physical property used in the calculation to determine the atomic ratio, H/Pd. Figure 6-1 describes the control volumes for the conservation of mass in the calculation of the atomic ratio.

![Figure 6.1 Diagram for the Calculation of the Atomic Ratio, H/Pd.](image)

Equations (6-7) through (6-14) are used to determine how the actual weight measurements of the hydrogen are included in the calculation of the atomic ratio.
The moles of the hydrogen within the three dashed line volumes of Figure 6.1 are constant. Thus, equation (6-7) is true:

\[ \text{mol}_1 + \text{mol}_2 + \text{mol}_3 = \text{constant} \]  \hspace{1cm} (6-7)

the moles of hydrogen in volume V2 are:

\[ \text{mol}_2 = \frac{P_2 V_2}{Z_2 RT_2} \]  \hspace{1cm} (6-8)

and the moles of hydrogen in volume V3 are:

\[ \text{mol}_3 = \frac{P_3 V_3}{Z_3 RT_3} \]  \hspace{1cm} (6-9)

In equation (6-7) "constant" is used for the total moles of hydrogen in the system, which remains constant throughout the experiment. Thus \( \text{mol}_1 \) is the moles of the hydrogen in the palladium solid plus the moles of the gaseous hydrogen in the volume 1 of the test bed. Equation (6-7), using (6-8) and (6-9) becomes equation (6-10), with \( \text{mol}_1 \) being split into two components. The two components of \( \text{mol}_1 \) are \( \text{mol}_{\text{H}_2 \text{ solid}} \) and the moles of the gaseous hydrogen, equation (6-7) becomes, at a specified temperature of 293.15K, equation (6-10):

\[
\text{constant} = (\text{mol}_{\text{H}_2 \text{ solid}} + \frac{P_1 V_1}{Z_1 R(293.15\text{K})}) + \frac{P_2 V_2}{Z_2 R(293.15\text{K})} + \frac{P_3 V_3}{Z_3 R(293.15\text{K})}
\]  \hspace{1cm} (6-10)

\( \text{mol}_{\text{H}_2 \text{ solid}} \) is the moles of hydrogen in the palladium solid. \( P \) is the pressure for each respective volume V. The "constant" is determined at a specific temperature. \( R \) is the universal gas constant. The weight measured in grams at 293.15°K divided by the molecular weight of hydrogen is equation (6-11):
The constant in equation (6-10) using (6-11) becomes equation (6-12):

$$\text{constant} = \frac{\text{weight measured at 293.15K}}{\text{MW}_{H_2}} + P\left(\frac{V_2}{Z_2 R(293.15K)} + \frac{V_3}{Z_3 R(293.15K)}\right)$$

(6-12)

The moles of the hydrogen in the solid can be found with the measured weight of the hydrogen, and the pressure, volume, and temperature inputs using equations (6-11) and (6-12) combined to form (6-13):

$$\text{mol}_{H_2\text{solid}} = \frac{\text{weight measured 293.13K}}{\text{MW}_{H_2}} + P\left(\frac{V_2}{Z_2 R(293.15K)} + \frac{V_3}{Z_3 R(293.15K)}\right) - P\left(\frac{V_1}{Z_1 R T_1} + \frac{V_2}{Z_2 R T_2} + \frac{V_3}{Z_3 R T_3}\right)$$

(6-13)

It must be noted that the $V_1$ is the volume of the dead space within the bed. As the palladium accepts hydrogen into the lattice, the palladium swells, thus reducing the volume of $V_1$. The reduction in the volume, $V_1$, is a direct function of the atomic ratio, $H/Pd$. Equation (6-14) is for the reduction in free volume due to the swelling of the palladium from (Wicke and Brodowsky, 1978).

$$\text{CorrectedVolume} = V_1 - \frac{(\text{Pd gm})(1.10777*(1+0.044*(H/Pd-0.607))^3 -1}{12.02 \frac{\text{gm Pd}}{\text{cm}^3}}$$

(6-14)

With equations (6-7) to (6-14) the atomic ratio can be calculated using the experimental weight measurement, the pressure, and temperature, and the known amount of palladium with equation (6-15):

$$\frac{H}{Pd} = \frac{2 \times \text{moles H}_2}{\text{moles Pd}}$$

(6-15)
The results of the experimentally measured atomic ratio are tabulated in the excel spreadsheet in Appendix A. The experimentally measured atomic ratio is in the plots of fugacity versus atomic ratio in Figures 6.2 and 6.3.

6.3 Plots of Fugacity Versus Atomic Ratio

The fugacity and the atomic ratio, H/Pd, can now be determined from the measured experimental data. The experimental data points for the temperatures -60°C, -40°C, -20°C, 0°C, 40°C, 60°C, 80°C, 100°C, and 120°C is plotted with the fugacity in psia versus the atomic ratio, H/Pd, in Figure 6.2. The curve fit to the data is also shown in Figure 6.2.

![Error bars are 0.5% on 40 deg C Isotherm](image)

Figure 6.2 Experimental Data of Fugacity versus Atomic Ratio, H/Pd.
The experimental data points and the curve fit for the 20°C isotherm are shown in Figure 6.3. The error bars at 40°C and 20°C represent the 0.5% error on the atomic ratio axis.

Figure 6.3 Experimental Data of Fugacity versus Atomic Ratio at 20°C.

Each of the isotherms in the experimental data shown in Figures 6.2 and 6.3 are curve fit to equation (6-16). The experimental constants, A and B, for the following curve fit are shown in Table 6.2.

\[ \ln f \text{ (psia)} = A(T) + B(T)(H/Pd) \]  

(6-16)
### Table 6.2 Constants for the Palladium-Hydrogen Curve fit.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>A</th>
<th>B</th>
<th>Temperature</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>-60°C</td>
<td>-46.547</td>
<td>61.85</td>
<td>40°C</td>
<td>-25.461</td>
<td>41.516</td>
</tr>
<tr>
<td>-40°C</td>
<td>-41.743</td>
<td>57.472</td>
<td>60°C</td>
<td>-20.631</td>
<td>39.075</td>
</tr>
<tr>
<td>-20°C</td>
<td>-36.206</td>
<td>51.99</td>
<td>80°C</td>
<td>-20.494</td>
<td>36.669</td>
</tr>
<tr>
<td>0°C</td>
<td>-32.269</td>
<td>48.242</td>
<td>100°C</td>
<td>-18.297</td>
<td>34.465</td>
</tr>
<tr>
<td>20°C</td>
<td>-28.502</td>
<td>44.487</td>
<td>120°C</td>
<td>-16.276</td>
<td>32.422</td>
</tr>
</tbody>
</table>

### 6.4 Comparison of Curve Fit With the Literature Data

The data for each isotherm of the palladium-hydrogen equation of state has been curve fit to the equation (6-16).

Wicke and Nernst, and Perminov, Orlov, and Frumkin have all experimented in the β-phase region. Their low temperature data is shown in comparison with the experimental curve fits in Figure 6.4, the error bars represent 1% error in the atomic ratio. Perminov, Orlov, and Frumkins’ experimental data was modified to express the pressure in terms of fugacity as shown in Appendix C.

Perminov, Orlov and Frumkins’ modified data at 0°C is within the 1% error in atomic ratio to a fugacity of 1000 psia, as shown in Figure 6.4. At this point Perminov, Orlov and Frumkins’ 0°C isotherm slopes up from this experimental curve fit. Perminov, Orlov and Frumkins’ modified low-pressure data at -32°C begins between the -40°C and the -20°C curve fits. Perminov, Orlov and Frumkins’ -32°C modified data then deviates from the curve fit of this study.
Comparison of Experimental Curve Fits with Wicke and Nernst, and Perminov, Orlov, Frumkin

Figure 6.4 Comparison of Low Temperature Experimental Curve Fits (Perminov, et al, 1952) and (Wicke and Nernst, 1964) with literature data.

Wicke and Nernst's -78°C and 0°C isotherms have the same general slope as the experimental isotherms in their vicinity. Wicke and Nernst's 0°C isotherm is offset from the curve fit of this study by 2%. Wicke and Nernst's 0°C isotherm is reads a higher atomic ratio than this study.

A comparison of Wicke and Nernst, and Perminov, Orlov and Frumkins' experimental data at -78°C is also shown in Figure 6.4. Perminov, Orlov and Frumkin noted that their data at this temperature was not very accurate.
A comparison of the higher temperature curve fits is shown in Figure 6.5. An error bar of 1% is shown on the experimental 40°C isotherm. All of Perminov, Orlov, and Frumkins’ modified data at 50°C are within 1% of the experimental curve fit.

Figure 6.5 Comparison of High Temperature Experimental Curve Fits (Perminov et al, 1952) and (Wicke and Nernst, 1964) with literature data.

Perminov, Orlov, and Frumkins’ 100°C modified data is within 1% of the experimental curve fit up to a fugacity of 1000 psia. At higher fugacities their 100°C isotherm has a lower atomic ratio than that shown by this study. Wicke and Nernsts’ 30°C and 50°C data are offset and read a higher atomic ratio by 2% than the experimental curve fit. This 2% offset in Wicke and Nernst’s data was seen in the low temperature data as well.
6.5 Uncertainty Analysis

The general uncertainty analysis that is employed for the estimating the uncertainty in the fugacity and the atomic ratio is the Kline-McClintock method (Holman, 1989). This method uses the products of the sensitivities of the measured variable with respect to the independent variables and the uncertainties of the independent variables themselves. The form of the uncertainty for fugacity becomes equation (6-17),

\[ U_f = \left[ \left( \frac{\partial f}{\partial p} \right)^2 U_p + \left( \frac{\partial f}{\partial T} \right)^2 U_T \right]^{\frac{1}{2}} \]  

(6-17)

Equation (6-18) is the partial derivative of fugacity with respect to pressure.

\[ \frac{\partial f}{\partial p} = \exp \left[ \left( C_0 + C_1 T + C_2 T^2 \right) \left( \frac{P}{T} \right) + \left( C_3 + C_4 T + C_5 T^2 \right) \left( \frac{P}{T} \right)^2 \right] \]

\[ + \left( C_6 + C_7 T + C_8 T^2 \right) \left( \frac{P}{T} \right)^3 \]  

(6-18)

Taking this partial derivative results in equation (6-19).

\[ \frac{\partial f}{\partial p} = \exp \left[ \left( C_0 + C_1 T + C_2 T^2 \right) \left( \frac{P}{T} \right) + \left( C_3 + C_4 T + C_5 T^2 \right) \left( \frac{P}{T} \right)^2 \right] \]

\[ + \left( C_6 + C_7 T + C_8 T^2 \right) \left( \frac{P}{T} \right)^3 \]  

(6-19)

\[ \left[ C_9 + C_{10} T + C_{11} T^2 \right] \left( \frac{P}{T} \right)^4 \]

\[ + \left[ C_{12} + C_{13} T + C_{14} T^2 \right] \left( \frac{P}{T} \right)^5 \]

\[ + \left[ C_{15} + C_{16} T + C_{17} T^2 \right] \left( \frac{P}{T} \right)^6 \]

\[ + \left[ C_{18} + C_{19} T + C_{20} T^2 \right] \left( \frac{P}{T} \right)^7 \]

The equation for the partial derivative of fugacity with respect to temperature is:
With these two partial derivatives and the uncertainty in sensitivities of the pressure and temperature the uncertainty in the fugacity can be determined. This is shown in the equation (6-21).

\[
\frac{\partial f}{\partial T} = P \left( \begin{array}{c}
- \frac{C_6 P}{T^2} + \frac{C_2 P}{T^3} - \frac{C_3 P^2}{2T^2} - \frac{C_4 P^2}{T^4} - \frac{C_6 P^3}{3(T^2)} \\
- \frac{C_8 P^3}{3(T^2)} - \frac{C_9 P^4}{T^5} - \frac{3}{4} \frac{C_{10} P^4}{T^4} - \frac{C_{11} P^4}{2T^3}
\end{array} \right) \times \\
\exp \left( \begin{array}{c}
[C_0 + C_1 T + C_2 T^2] \frac{P}{T} + [C_3 + C_4 T + C_5 T^2] \frac{1}{2} \left( \frac{P}{T} \right)^2 \\
+ [C_6 + C_7 T + C_8 T^2] \frac{1}{3} \left( \frac{P}{T} \right)^3 + [C_9 + C_{10} T + C_{11} T^2] \frac{1}{4} \left( \frac{P}{T} \right)^4
\end{array} \right) \times
\left[ \begin{array}{c}
\left[ C_0 + C_1 T + C_2 T^2 \right] \frac{P}{T} + \left[ C_3 + C_4 T + C_5 T^2 \right] \frac{1}{2} \left( \frac{P}{T} \right)^2 \\
\exp \left[ \frac{C_6 + C_7 T + C_8 T^2}{P} \right] \frac{1}{3} \left( \frac{P}{T} \right)^3 + \left[ C_9 + C_{10} T + C_{11} T^2 \right] \frac{1}{4} \left( \frac{P}{T} \right)^4
\end{array} \right)
\]
The general uncertainty analysis in the determination of the atomic ratio is calculated in terms of the uncertainty in the moles of hydrogen. Equation (6-22) is the general equation for the uncertainty in the moles of hydrogen.

\[
U_{\text{mol} \text{H}_2} = \left[ \left( \frac{\partial \text{mol} \text{H}_2}{\partial \text{weight}} U_{\text{weight}} \right)^2 + \left( \frac{\partial \text{mol} \text{H}_2}{\partial P} U_P \right)^2 + \left( \frac{\partial \text{mol} \text{H}_2}{\partial V_1} U_{V_1} \right)^2 + \left( \frac{\partial \text{mol} \text{H}_2}{\partial V_2} U_{V_2} \right)^2 \right]^{\frac{1}{2}}
\]

(6-22)

Equations for the partial derivatives involved in the determination of the uncertainty in the moles of hydrogen are shown in equations (6-23) thru (6-28)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial \text{weight}} = \frac{1}{MW_{\text{H}_2}}
\]

(6-23)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial P} = \left( \frac{V_2}{Z_2RT_2} + \frac{V_3}{Z_3RT_3} \right)_{\text{20degC}} - \left( \frac{V_1}{Z_1RT_1} + \frac{V_2}{Z_2RT_2} + \frac{V_3}{Z_3RT_3} \right)
\]

(6-24)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial V_1} = -\frac{P}{ZRT_1}
\]

(6-25)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial V_2} = \left( \frac{P}{Z_2RT_2} \right)_{\text{20degC}} - \frac{P}{Z_2RT_2}
\]

(6-26)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial V_3} = \left( \frac{P}{Z_3RT_3} \right)_{\text{20degC}} - \frac{P}{Z_3RT_3}
\]

(6-27)

\[
\frac{\partial \text{mol} \text{H}_2}{\partial T_{1,2}} = \left( -\frac{PV_1}{Z_1RT_1^2} U_{T_1,2} \right)
\]

(6-28)
\[
\frac{\partial \text{mol } H_2}{\partial T_3} = \left( -\frac{PV_3}{Z_3RT_3^2} \right)_{20 \text{degC}} + \frac{PV_3}{Z_3RT_3^2}, \quad (6-29)
\]

The partial derivatives are inserted into the general uncertainty equation (6-22). The uncertainty in the moles of hydrogen can now be calculated using measured experimental quantities. With the collective equations (6-23) to (6-29) the uncertainty in the moles of hydrogen is stated in equation (6-30).

\[
U_{\text{mol } H_2} = \left( \frac{1}{MW_{H_2}} U_{\text{weight}} \right)^2 + \left( \left( \frac{P}{Z_1RT_1} U_{T_1} \right)^2 + \left( \left( \frac{P}{Z_2RT_2} \right)_{20 \text{degC}} - \left( \frac{P}{Z_2RT_2} \right) U_{T_2} \right)^2 + \left( \left( \frac{P}{Z_3RT_3} \right)_{20 \text{degC}} - \left( \frac{P}{Z_3RT_3} \right) U_{T_3} \right)^2 \right)^{\frac{1}{2}}.
\quad (6-30)
\]

The calculation for the uncertainty in the atomic ratio is derived from the definition of the atomic ratio, which is shown in equation (6-31).

\[
\frac{H}{\text{Pd}} = \frac{2 \cdot \text{mols } H_2}{\text{mols Pd}}, \quad (6-31)
\]

The uncertainty in the atomic ratio of hydrogen to palladium can be calculated with respect to the independent variables, moles of hydrogen and moles of palladium. Utilizing the uncertainty in the moles of hydrogen found in equation (6-30) and knowing the uncertainty in the moles of palladium, the uncertainty of the atomic ratio can be
calculated. The calculation for the uncertainty in the atomic ratio is shown in equation (6-32).

\[
U_{\frac{H}{Pd}} = \left( \frac{2}{\text{mol Pd}} U_{\text{mol H}_2} \right) + \left( \frac{2 \cdot \text{mol H}_2}{(\text{mol Pd})^2} U_{\text{mol Pd}} \right)^2 \right)^{1/2}
\]

(6-32)

The uncertainty in the atomic ratio is calculated for each of the individual atomic ratio data points, shown in Appendix A. A determination of the largest effect on the uncertainty in the atomic ratio was done by selectively zeroing the sensitivities of the each of the independent variables in the general uncertainty equation. The largest effect on the uncertainty of the atomic ratio is the uncertainty in the moles of hydrogen. This uncertainty is greatly affected by the sensitivity in the weight measurement. The uncertainty is larger for the palladium beds that have a low pressure and thus a lower mass of hydrogen. Conversely the uncertainty is smaller with high pressures and higher loads of hydrogen because of the higher weight of hydrogen. For instance the uncertainty at room temperature and 660 psia is 0.3% of the atomic ratio and at room temperature and 10,000 psia the uncertainty is 1.2% of the atomic ratio.

The sensitivity of the pressure transducers has the second largest effect on the uncertainty of our measurements. In this experiment many different ranges of the Heise pressure transducers are used. The sensitivity is quoted by the manufacturer to be better than ±0.005 of the span. The higher the range of the transducer the higher the uncertainty in the measurement. The pressure transducers were matched with each loading of the palladium bed to try to reduce unnecessary uncertainty in the measurements.
CHAPTER 7

Conclusions and Recommendations

7.1 Conclusions and Recommendations

This study demonstrates that taking a direct gravimetric weight measurement of a 50 gram hydrided palladium bed is a viable and accurate method of determining the equation of state for the palladium-hydrogen system. Curve fit data has been determined for the atomic ratio from -60°C to 120°C with a range in pressures of 0 to 20,000 psia.

The uncertainty of the measurement of the atomic ratio, H/Pd, is greatly influenced by the sensitivity, accuracy, and method of taking the weight measurement of the hydrided palladium bed. The largest contributor to the uncertainty is the sensitivity of the weight measurement. An increase in the accuracy and precision of the mass balance would further improve the results of a future experiment. The accuracy and precision of the pressure measurement is a secondary contributor to the uncertainty of the measurement. An improvement in the accuracy of the pressure transducers would improve the accuracy of the measurements. This improvement would not have as large an effect as an improvement in the weight measurement.

The accuracy in the determination of the equation of state of the palladium was improved upon in this investigation. The data was curve fit to a known equation used in the literature and 95% fugacity versus atomic ratio data points lie within 1% of the curve fit. The error in the data lie within the calculated uncertainty of the atomic ratio.

The experimental curve fit was compared to the literature. The experimental curve fit is within 1% of the atomic ratio of Perminov, Orlov, and Frumkins' data in the pressure region below 1,000 psia. Above this pressure Perminov, Orlov and Frumkins'
data slopes up and away from the experimental correlation. Wicke and Nernst's' data is also compared to this correlation and was found to have an atomic ratio that is 2% higher than this studies data. Factors that could cause this offset in the atomic ratio are impurities in the system, impurities in the palladium or hydrogen, or a systematic error in the volumetric method used by Wicke and Nernst.

An extension of this work could include the determination of the palladium-deuterium, palladium-tritium, metal-hydride equations of state. Other future work in this area could be to extend the pressure and temperature limits to determine if the experimental correlation could accurately predict the palladium-hydrogen equation of state in these ranges.
APPENDICIES

A. Raw Excel Data Sheets................................................................. 53
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### Compressibility constants

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### Moles in the gas phase

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<th>Fugacity</th>
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### PCT Constants, Meyer 1995

For the equation \( \ln(a-(b-cn)/T-dT) \)

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### Moles in the gas phase

- **Fugacity**
- **mole**
- **H/Pd**
- **Free bed**
- **Tainty**

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for the equation \( \ln f = a - (b - cn)/T - dT \)

#### PCT Constants, Meyer 1995

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### PCT Constants, Meyer 1995

For the equation \( \ln f = a - (b - cn) / T - dT \)

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### Units were opened with a half turn

<table>
<thead>
<tr>
<th>V1 cc</th>
<th>V2 cc</th>
<th>V3 cc</th>
<th>X-Ducer unit (gm)</th>
<th>weight of before load</th>
<th>weight of load in grams</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.302</td>
<td>50.1167</td>
<td>0.173</td>
<td>H 25855</td>
<td>1648.465</td>
<td>1648.797</td>
</tr>
<tr>
<td>6.394</td>
<td>50.5392</td>
<td>0.173</td>
<td>H 27164</td>
<td>1645.12</td>
<td>1645.446</td>
</tr>
<tr>
<td>6.427</td>
<td>50.5348</td>
<td>0.173</td>
<td>H 25854</td>
<td>1635.168</td>
<td>1635.484</td>
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<tr>
<td>6.381</td>
<td>50.5204</td>
<td>0.173</td>
<td>H 25851</td>
<td>1653.087</td>
<td>1653.393</td>
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<tr>
<td>6.367</td>
<td>50.5015</td>
<td>0.173</td>
<td>P 60828</td>
<td>1658.495</td>
<td>1658.797</td>
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</tbody>
</table>

### Moles in the gas phase

<table>
<thead>
<tr>
<th>Date</th>
<th>time</th>
<th>unit</th>
<th>Pressure psia</th>
<th>Temp bed ºC</th>
<th>Temp out ºC</th>
<th>H2 solid</th>
<th>H/Pd</th>
<th>% Uncert</th>
</tr>
</thead>
<tbody>
<tr>
<td>3/10/98</td>
<td>9:32</td>
<td>1</td>
<td>299.56</td>
<td>121.42</td>
<td>23.6</td>
<td>0.00363</td>
<td>0.00011</td>
<td>0.00129</td>
</tr>
<tr>
<td>178.73</td>
<td>120.9</td>
<td>24.3</td>
<td>0.00218</td>
<td>0.00006</td>
<td>0.00246</td>
<td>179.79</td>
<td>0.157084</td>
<td>0.66142</td>
</tr>
<tr>
<td>3</td>
<td>100.54</td>
<td>120.9</td>
<td>24.3</td>
<td>0.00123</td>
<td>0.00004</td>
<td>0.00139</td>
<td>100.87</td>
<td>0.154118</td>
</tr>
<tr>
<td>56.4</td>
<td>120.62</td>
<td>24.1</td>
<td>0.00070</td>
<td>0.00002</td>
<td>0.00078</td>
<td>56.51</td>
<td>0.150152</td>
<td>0.63247</td>
</tr>
<tr>
<td>32.37</td>
<td>120.2</td>
<td>24</td>
<td>0.00040</td>
<td>0.00001</td>
<td>0.00007</td>
<td>32.40</td>
<td>0.145996</td>
<td>0.61519</td>
</tr>
<tr>
<td>3/10/98</td>
<td>11:26</td>
<td>1</td>
<td>198.92</td>
<td>100.96</td>
<td>23.6</td>
<td>0.00255</td>
<td>0.00008</td>
<td>0.00086</td>
</tr>
<tr>
<td>2</td>
<td>113.86</td>
<td>100.6</td>
<td>24.2</td>
<td>0.00147</td>
<td>0.00004</td>
<td>0.00157</td>
<td>114.31</td>
<td>0.158709</td>
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<td>3</td>
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<td>0.00002</td>
<td>0.00080</td>
<td>57.88</td>
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</tr>
<tr>
<td>4</td>
<td>29.55</td>
<td>100.43</td>
<td>24.2</td>
<td>0.00038</td>
<td>0.00001</td>
<td>0.00041</td>
<td>29.58</td>
<td>0.150844</td>
</tr>
<tr>
<td>7</td>
<td>15.813</td>
<td>100.1</td>
<td>24.2</td>
<td>0.00021</td>
<td>0.00001</td>
<td>0.00003</td>
<td>15.82</td>
<td>0.146232</td>
</tr>
</tbody>
</table>
program fill2

 implicit none
 real*8 a(3), b(3), c(3), d(3), e(75), rr, r, k, sf(3,3), temp, tempa, 1
 phi, ptot, pold, mb(5), mbop(5), mbs(5), x(5), mpd, mt20b, mhe30b, 2
 tempa, phi, ptot, pold, mb(5), mbop(5), mbs(5), x(5), mpd, mt20b, mhe30b, 3
 delp, zeff, vb, vrep, delp, zeff, vb0, mfn, nall, pall, yold, YY(3), 4
 tmp1, tmp2, tmp3, tmp4, tmp5, tmp6, tmp7, tmp8, tmp9, tmp10, tmp11, 5
 deld, delt, yold, yoldt, dtexp, sall, ball, calll, calll, calll, calll, calll, 6
 a, y(5), tot, 7
 cc(5), dd(5), ee(5), ff(5), gg(5), a1, a2, a3, a4, a5, delt, zold 8
 integer igas, irnep 9
 character*30 tmp 10
 character*1 good 11
 data a / 5.83, 32.39, 28.49 / ! PCT constants 12
 data b /12640., 15313., 1.5349. / ! PCT constants 13
 data c /12832., 12832., 1.3572. / ! PCT constants 14
 data d /0.01853, -.0327, -.02363 / ! PCT constants 15
 data e/ 1 .022456, 8.3057e-4, -1.0193e-6, 2 .056181, -1.9111e-4, 3 .5657e-7, 3 .036149, -8.1655e-6, 4 .0139e-8, 4 -1.5121e-4, 2.7545e-6, -4.6721e-9, 5
 character*30 tmp 6
 character*1 good 7
 data a / 5.83, 32.39, 28.49 / ! PCT constants 8
 data b /12640., 15313., 1.5349. / ! PCT constants 9
 data c /12832., 12832., 1.3572. / ! PCT constants 10
 data d /0.01853, -.0327, -.02363 / ! PCT constants 11
 data e/ 1 .022456, 8.3057e-4, -1.0193e-6, ! Z constants a1 H2 2 .056181, -1.9111e-4, 1.5657e-7, ! Z constants a2 3 .036149, -8.1655e-6, 3.0139e-8, ! Z constants a3 4 -1.5121e-4, 2.7545e-6, -4.6721e-9, ! Z constants a4

...
Appendix B

```
H2
0,0,0,

D2
1 0.06214289821e-4,-1.1201e-6,
2 0.058847-2.1402e-4,2.0254e-7,

D2
3 -0.004784713188e-6,1.2312e-8,
4 -1.388e-5,1.6842e-6,-2.7094e-9,

D2
5 0,0,0,

T2
1 -2.109e-5,9.2529e-4,-1.1593e-6,
2 0.06076,-2.2813e-4,2.273e-7,

T2
3 -0.005349,6.8348e-6,2.7755e-9,
4 7.1281e-5,1.0614e-6,-1.6328e-9,

T2
5 0,0,0,

He-3
1 .15849,-2.6866e-5,-5.2201e-8,
2 .0018328,-4.0134e-5,5.8146e-8,

He-3
3 -5.2376e-4,5.0454e-6,-6.9967e-9,
4 6.6813e-6,-2.3159e-8,-2.0797e-10,

He-3
5 0,0,0,

N2
1 -1.7618,0.0085229,-9.695e-6,
2 1.3616,-0.0053109,6.0426e-6,

N2
3 -0.35382,0.01251,-1.3966e-6,
4 0.37694,-1.0501e-4,1.1648e-7,

N2
5 -0.0096532,-2.4486e-7,0.

rr = 1.9872
al/gmole |K
r = 82.057
|K
k = 0.056216
zold=1.0

gas constant c
|cm^3 atm/gmole

dk constant 1/year

read & confirm input file

call r-cad input (mb,vb,vrrep,tempa,mpd,mfn,dtemp,y,tot)
good(1:1) = 'N'
write(6,*),'Are these parameters correct [y or n]?'
read(5,*) good
if (good(1:1) .eq. 'n' .or. good(1:1) .eq. 'N') then
write(6,*),'Please edit the file delivery.inp and restart'
goto 999
endif

call initialize (mb,mbop,mt20b,mhe30b,ptot,pall,tempa,vb0,vb,YY,y,
1 aall,ball,calll,dall,a,b,c,d,cc,dd,ee,ff,gg,x,zeff,a1,a2,a3,a4,a5,
```
Appendix B

e) 

cc

open output file fill2.out
cc

open(unit=2, file='fill2.out1', status='unknown')
cc

write headers for output
cc

write(6, 910) ' stoic(all) ptot(psia) pTDH(psia) mbs(H2) mbop(H2) vb(cc)
write(2, 910) ' stoic(all) ptot(psia) pTDH(psia) mbs(t2) mbop(t2) vb(cc)
cc
determine stoic given P & T
cc

1 temp = tempa + dtemp  ! bed temp. with self heating
sf(2,1) = exp(277.5/temp - 0.025)  ! deuterium/protium separation factor
sf(3,1) = exp(430.4/temp - 0.092)  ! tritium/protium separation factor
sf(3,2) = exp(133.5/temp - 0.021)  ! tritium/deuterium separation factor
sf(1,2) = 1/sf(2,1)  ! protium/deuterium separation factor
sf(1,3) = 1/sf(3,1)  ! protium/tritium separation factor
sf(2,3) = 1/sf(3,2)  ! deuterium/tritium separation factor

phi = al*(ptot/temp)+a2*(ptot/temp)**2/2+a3*(ptot/temp)**3/3+a4*(ptot/temp)**4/4

phi = phi + a5*(ptot/temp)**5/5

phi = exp(phi)  ! fugacity coefficient

write(6, *) 'phi=',phi

tmp1 = aall-ball/temp+all*temp
nall = min*(log(pall*phi)-tmp1)*temp/calll  ! total stoic

! total moles tritium

! plateau pressure atm

if ((pall - tmp2) < 0.001.) then
vb = vb0 - (mpd*106.4/12.02)*nall*(.179*x(3) + .182*x(2) + .185*x(1))
nall = 2*(mb(1) + mb(2) + mb(3) - tmp2*(vb+vrep)/(zeff*r*temp))/mpd
endif

2 continue

determine the pressure in the system

! total moles helium

mb = mhe30b  ! total moles helium
vb = vb0 - (mpd*106.4/12.02)*nall*(.179*x(3) + .182*x(2) + .185*x(1))
do 16 i = 1,3
mb(i) = x(i)*nall*mpd/2.0  ! hydrogen solid
16 continue

mb(4) = 0.
do 18 i = 1,4
mbop(i) = mb(i) - mbs(i)  ! moles overpresure
18 continue
Appendix B

```plaintext
sum moles of gas
moptot = 0.0
do 20 igas = 1,5
   moptot = moptot + mbop(igas)   ! moles total gas
s
20 continue
a1 = 0
a2 = 0.
a3 = 0.
a4 = 0.
a5 = 0.
if(moptot .le. 0) then
   ptot=tmp2
   pall=tmp2
   goto1
endif
nep = 1
do 40 i = 1,5
   cc(i) = e(nep) + e(nep+1)*temp + e(nep+2)*temp**2  !
   dd(i) = e(nep+3) + e(nep+4)*temp + e(nep+5)*temp**2  !
   ee(i) = e(nep+6) + e(nep+7)*temp + e(nep+8)*temp**2  !
   ff(i) = e(nep+9) + e(nep+10)*temp + e(nep+11)*temp**2 !
   gg(i) = e(nep+12) + e(nep+13)*temp + e(nep+14)*temp**2 !
40 nep = 5*3*i + 1

101 zeff = 1 + a1*(ptot/temp)+a2*(ptot/temp)**2+a3*(ptot/temp)**3+a4*(ptot/temp)**4  !
   zeff = zeff + a5*(ptot/temp)**5
   ptot = zeff*(moptot*r*temp)/(vb*vrep)   ! atm
   del = abs((zeff-zold)/zold)
   zold = zeff
write(6,*) 'nall,zeff,ptot,pall=',nall,zeff,ptot,pall
if(del .gt. .0001) goto 101
aa = call1/temp
nall = 2*(mb(1) + mb(2) + mb(3) - pall*(vb+vrep)/(zeff*r*temp) )/mpd
if ((pall - tmp2) .lt. .002) pall = tmp2 !plateau pressure
1   ((vb+vrep)/(zeff*r*temp) + mpd/(pall*2.0*aa))  !partial hydrogen pressure
   pall = (rob(l) + rob(2) + rob(3) + (1/aa - nall)*mpd/2.0)/
   ((vb+vrep)/(zeff*r*temp) + mpd/(pall*2.0*aa))  ! partial hydrogen pressure
   phi = al*(ptot/temp)+a2*(ptot/temp)**2/2+a3*(ptot/temp)**3/3+a4*(ptot/temp)**4/4
   phi = phi + a5*(ptot/temp)**5/5
   phi = exp(phi)   ! fugacity coefficient
   nall=mn*(log(pall*phi) - tmp1)*temp/call1
   if ((pall - tmp2) .lt. 0.002) then
      pall=tmp2
   endif
   pall = 2*(mb(1) + mb(2) + mb(3) - pall*(vb+vrep)/(zeff*r*temp))/mpd
   pall = 2*(mb(1) + mb(2) + mb(3) - pall*(vb+vrep)/(zeff*r*temp))/mpd
   pall = (rob(l) + rob(2) + rob(3) + (1/aa - nall)*mpd/2.0)/
   ((vb+vrep)/(zeff*r*temp) + mpd/(pall*2.0*aa))  !partial hydrogen pressure
   if ((pall - tmp2) .lt. .002) pall = tmp2 !plateau pressure
   if (delp .gt. 0.0001) goto 2
   endif
   if (delp .gt. 0.0001) goto 2
   endif
   endif
   endif
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   endif
   endif
   ```
```
Appendix B

solving for fraction of protium in gas phase

c

c

c

c

c

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c

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tritium in gas phase

c

c

c

deuterium in gas phase

c

c

c

protium, deuterium & tritium in solid phase

c

c

c

protium, deuterium & tritium in solid phase

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Appendix B

\[ x(1) = \frac{YY(1)}{YY(1) + sf(1,2) \cdot YY(2) + sf(1,3) \cdot YY(3)} \]
\[ x(2) = \frac{YY(2)}{YY(2) + SE(2,3) \cdot YY(3) + sf(2,1) \cdot YY(1)} \]
\[ x(3) = \frac{YY(3)}{YY(3) + sf(3,1) \cdot YY(1) + sf(3,2) \cdot YY(2)} \]

calculate new constants for PCT
c
\[ a_{all} = 0.0 \]
\[ ball = 0.0 \]
\[ calll = 0.0 \]
\[ dall = 0.0 \]
do 310 i = 1,3
\[ a_{all} = x(i) \cdot a(i) + a_{all} \]
\[ ball = x(i) \cdot b(i) + ball \]
\[ calll = x(i) \cdot c(i) + calll \]
\[ dall = x(i) \cdot d(i) + dall \]
310 continue

cconvergence check
deld = abs(yoldd - YY(2))
yoldd = YY(2)
delt = abs(yoldt - YY(3))
yoldt = YY(3)
if(deld . gt. 0.00001) goto 1
if(delt . gt. 0.00001) goto 1
write(6,*,'converged on bed')
write(6,900) nall,ptot*14.696, pall*14.696, mbs, mbop, vb, phi*ptot
write(2,900) nall,ptot*14.696, pall*14.696, mbs, mbop, vb, phi*ptot
close(unit=2)
900 format(10e12.5)
910 format(a80)
999 stop
end

subroutine read input(mb,vb,vrep,tempa, mpd, mfn, dtemp, y, tot)
implicit none
teal*8 rob(l), vb,vrep, tempa, mpd, mfn, dtemp, y(l), tot
character*30 tmp
integer igas
ccc hydrogen, igas = 1
ccc deuterium, igas = 2
ccc tritium, igas = 3
ccc helium 3, igas = 4
ccc others, igas = 5
ccc read inputs from file fill2.inp
Appendix B

```fortran
open(unit=1, file='fill2.inp', status='old')
c bed gas call skip call skip call skip
tot = 0.
do 110 igas = 1,5
   read(1,*) mb(igas), tmp
   write(6,*) mb(igas), tmp
   tot = mb(igas) + tot
110 continue
do 100 igas = 1,5
   y(igas) = mb(igas)/tot
   write(6,*) y(igas)
100 continue
c Volumes call skip call skip call skip
   read(1,*) vb, tmp
   write(6,*) vb, tmp
   call skip
   read(1,*) vrep, tmp
   write(6,*) vrep, tmp
   call skip
   read(1,*) tempa, tmp
   write(6,*) tempa, tmp
   call skip
   read(1,*) dtemp, tmp
   write(6,*) dtemp, tmp
   call skip
   read(1,*) mpd, tmp
   mpd=mpd/106.4
   write(6,*) mpd, tmp
   call skip
   read(1,*) mfn, tmp
   write(6,*) mfn, tmp
   call skip
   close (unit = 1)
return
end
```

...and so on.
Appendix B

e)

```fortran
implicit none
real*8 mb(1), mbop(1), mt20b, mhe30b, ptot, pall, tempa, vb0, vb, YY(l), aall,
ball,
1 call1, dall, a(l), b(l), c(l), d(l), cc(l), dd(l), x(l), zeff, a1, a2, a3, a
4, a5, e(l),
2 ee(l), ff(l), gg(l), y(l)
integer l, nep
```

```
initial conditions
```

```
zeff=1.
mt20b = mb(3)
mhe30b = mb(4)
ptot = 50.0 ! atm total pressure
pall = ptot
mbop(5) = mb(5)
tempa = tempa + 273.15
vb0 = vb
aall = 0.
bball = 0.
call1 = 0.
dall = 0.
do 10 i=1, 3
YY(i) = mb(i)/(mb(1)+mb(2)+mb(3))
x(i) = YY(i)
aall = x(i)*a(i) + aall
ball = x(i)*b(i) + ball
call1 = x(i)*c(i) + call1
dall = x(i)*d(i) + dall
10 continue
nep = 1
```

```
do 40 i = 1, 5
cc(i) = e(nep) + e(nep+1)*tempa + e(nep+2)*tempa**2 !
dd(i) = e(nep+3) + e(nep+4)*tempa + e(nep+5)*tempa**2 !
ee(i) = e(nep+6) + e(nep+7)*tempa + e(nep+8)*tempa**2 !
ff(i) = e(nep+9) + e(nep+10)*tempa + e(nep+11)*tempa**2 !
gg(i) = e(nep+12) + e(nep+13)*tempa + e(nep+14)*tempa**2 !
40 nep = 5*3*i + 1
a1 = 0.
a2 = 0.
a3 = 0.
a4 = 0.
a5 = 0.
do 30 i = 1, 5
a1 = a1 + cc(i)*y(i)
a2 = a2 + dd(i)*y(i)
a3 = a3 + ee(i)*y(i)
a4 = a4 + ff(i)*y(i)
a5 = a5 + gg(i)*y(i)
30 continue
return
end
```
### Data From Wicke and Nernst, and Perminov, Orlov and Frumkin

<table>
<thead>
<tr>
<th>Press (psia)</th>
<th>H/Pd (calc)</th>
<th>Wicke and Nernst</th>
<th>Pressure (atm)</th>
<th>Fugacity (Meyer)</th>
<th>H/Pd</th>
<th>H/Pd</th>
<th>H/Pd</th>
<th>H/Pd</th>
<th>H/Pd</th>
<th>H/Pd</th>
</tr>
</thead>
<tbody>
<tr>
<td>-78.5</td>
<td>52.9124247</td>
<td>66.4</td>
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REFERENCES


Berichte der Bunsengesellschaft, 68, 224-235.
