Integrating the H₂ Extracted from the Still

C. Steven Whisnant

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Abstract

When starting the distillery, the concentration of H₂ is monitored by the residual gas analyzer (RGA) both to determine that the still is working and to determine at what point the H₂ has been substantially removed and the gas can be collected as good HD. One tool for determining this switch-over point is an extrapolation of the integrated H₂ content of the gas extracted. This document explains how this integration is done.

1 Computing the Total H₂ Content in the Gas

The total amount of gas extracted from the still is determined by the pressure of the gas put into one of the two-mole tanks on the still. Since the tank holds 2 moles at 1 ATM, the number of moles of gas extracted from the still, \( M_e \) is given by

\[
M_e(P) = \left( \frac{2 \text{ moles}}{10^3 \text{ mB}} \right) \cdot P
\]

(1)

Anticipating where we are going, this equation can be rewritten as an integral

\[
M_e(P) = \left( \frac{2 \text{ moles}}{10^3 \text{ mB}} \right) \int_0^P p \, dp
\]

(2)

Writing it this way makes it easy to shift our focus from the total amount of gas extracted to the the amount of H₂ extracted. For this we must multiply by the fraction of the total that is H₂. Since this changes as the pressure changes, we must include the fraction of H₂ in the gas under the integral. The fraction of H₂ in the gas is \( \frac{[\% \text{H}_2(p)]}{10^2} \) so the integral becomes

\[
M^{H_2}_e(P) = \left( \frac{2 \text{ moles}}{10^3 \text{ mB}} \right) \int_0^P \frac{[\% \text{H}_2(p)]}{10^2} p \, dp
\]

(3)

2 Computing the Total Fraction of H₂

The next step is compute the total amount of H₂ in the still. This is simply the measured fraction of H₂ in the raw HD multiplied by the total amount of gas. If the raw fraction is \( f_r^{H_2} \) and the total number of moles in the still is \( M_t \), then the total amount of H₂ in the still is

\[
M^{H_2}_t = M_t \cdot f_r^{H_2}
\]

(4)

The fraction of H₂ in the raw gas is given in terms of the percentage as

\[
f_r^{H_2} = \frac{[\% \text{H}_2]}{10^2}
\]

(5)

so that

\[
M^{H_2}_t = M_t \cdot \frac{[\% \text{H}_2]}{10^2}
\]

(6)
3 Putting it all Together

Now we can compute the fraction of the total amount of \( H_2 \) in the gas that has been extracted by forming the ratio of the two above quantities

\[
f_t^{H_2}(P) = \frac{M_t^{H_2}(P)}{M_t^{H_2}}
\]  

(7)

Substituting on the right hand side gives

\[
f_t^{H_2}(P) = \left(\frac{2 \text{ moles}}{10^3 \text{ mB}}\right) \int_0^P \frac{[\%H_2(p)]}{10^2} dp
\]

or

\[
f_t^{H_2}(P) = \left(\frac{2 \text{ moles}}{10^3 \text{ mB}}\right) \int_0^P \frac{[\%H_2(p)]}{M_t \cdot [\%H_2]} dp
\]

(8)

(9)

Since the typical \( H_2 \) content of the raw gas is 2\% and 12 moles of gas are in the still we get

\[
f_t^{H_2}(P) = \left(\frac{2 \text{ moles}}{10^3 \text{ mB}}\right) \frac{\int_0^P [\%H_2(p)] dp}{12 \text{ moles} \cdot 2}
\]

(10)

which reduces to

\[
f_t^{H_2}(P) = \left(\frac{1}{1.2 \times 10^4 \text{ moles} \text{ mB}^{-1}}\right) \int_0^P [\%H_2(p)] dp
\]

or

\[
f_t^{H_2}(P) = 8.3 \times 10^{-5} \text{ moles mB}^{-1} \int_0^P [\%H_2(p)] dp
\]

(11)

(12)

4 Doing it Numerically

Since we want to compute the integral as a function of the integral’s upper limit, it is best to use Euler’s method rather than one of the more precise methods usually coded for more serious work. This method is easy to implement in a spreadsheet.

To set this up in a spreadsheet, first define cell with the following labels and contents:

**Tank\_Capacity** This cell contains the contents of a single tank on the manifold in units of moles. Normally, this is 2.0.

**Full\_Pressure** This is the pressure in mB when the manifold tank actually contains the amount given in **Tank\_Capacity**. This is normally \( 10^3 \).

**Convert\_Precent** This is the conversion factor from percent to fraction. This should be \( 10^2 \).

**Moles\_in\_Still** This is total amount of gas in the still for this run. The units are moles.

**Bulk\_H2\_Percent** This is the measured percentage of \( H_2 \) in the raw HD gas.

With these definitions in hand, we can create the following useful combinations of variables for display purposes here.

\[
a = \frac{\text{Tank\_Capacity}}{\text{Full\_Pressure}}
\]

\[
b = \frac{\text{Convert\_Precent}}{\text{Moles\_in\_Still} \cdot \text{Bulk\_H2\_Percent}}
\]  

(13)
Table 1: Spreadsheet setup for computing the fraction of H\textsubscript{2} extracted from the still.

<table>
<thead>
<tr>
<th>P\textsubscript{man}</th>
<th>%H\textsubscript{2}</th>
<th>dp</th>
<th>Integral</th>
<th>Ext. (moles)</th>
<th>Frac. Ext.</th>
</tr>
</thead>
<tbody>
<tr>
<td>p\textsubscript{0}</td>
<td>%0</td>
<td>dp\textsubscript{0} = 0</td>
<td>(I_0 = 0)</td>
<td>(M_0 = aI_0)</td>
<td>(f_0 = bM_0)</td>
</tr>
<tr>
<td>p\textsubscript{1}</td>
<td>%1</td>
<td>dp\textsubscript{1} = (p\textsubscript{1} - p\textsubscript{0})</td>
<td>(I_1 = \frac{p\textsubscript{1} \times \text{percent}}{\text{convert percent}} + I_0)</td>
<td>(M_1 = aI_1)</td>
<td>(f_1 = bM_1)</td>
</tr>
</tbody>
</table>

Then columns can be created as shown in table 1. Once this is created, then the second row of the table can be copied down the page to do the integral.

It is then useful to create two plots in the spreadsheet. First, a graph showing the %H\textsubscript{2} versus P\textsubscript{man} so that the operation of the still is easy to follow. Secondly, a graph of the fraction extracted versus P\textsubscript{man} can be used to extrapolate to a fraction of one to find the amount of gas that must be extracted before switching manifold tanks and calling the gas “good HD”.