Accuracy of BGA244 for measuring diborane in hydrogen (using nitrogen as a proxy for diborane)
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Diborane (B₂H₆, CAS # 19287-45-7) is used as a p-type dopant in semiconductor processing. Because it is unstable in its pure form, diborane is sold as a compressed gas diluted in hydrogen. This study was carried out to assist an industrial gas supplier who wanted to use the BGA244 to measure the mole fraction of diborane in hydrogen.

Diborane caches fire and forms explosive mixtures when exposed to air and can be fatal if inhaled. Because of this, the BGA244 Binary Gas Analyzer was evaluated for this application using nitrogen as a safe proxy for diborane. Diborane and nitrogen have comparable atomic weights (27.76 and 28.01) and comparable speeds of sound (320 m/s and 349 m/s at NTP) and so behave comparably in the BGA244.

The BGA244’s Gas Table has the thermodynamic constants for hydrogen, nitrogen, diborane, as well as about 500 other liquids and gases, enabling the analysis of tens of thousands of mixtures.

A simple arrangement was used to test the BGA244 over a wide range of mixtures: The BGA244’s 130 cc acoustic cavity was filled with pure nitrogen, allowed to settle, data recording was started, and after 10 seconds a flow of 20 sccm of hydrogen was started. To prevent backflow, the cavity was vented through a narrow tube into the room at 14.7 psia. The hydrogen flow purged the cell of nitrogen, exponentially converging to pure hydrogen with a time constant of 130 cc/20 sccm= 6.5 minutes.

Actually data from the scan is graphed below:
Analytic fit to exponential mixing

For \( t \geq t_0 \), the mole fraction of nitrogen was expected to follow this equation:

\[
\text{Mole fraction of nitrogen}(t) = A \cdot e^{-(t-t_0)/\Gamma}
\]

We used \( A = 100\% \), \( t_0 = 10 \text{ s} \) and \( \Gamma = 6.5 \text{ minutes} = 390 \text{ seconds} \) as initial estimates. Excel’s Solver fit this equation to the measured mole fraction of nitrogen vs. time to improve on these initial estimates, finding \( A = 99.992 \% \), \( t_0 = 9.152 \text{ s} \) and \( \Gamma = 376.504 \text{ s} \).

With the assumption that the system conforms to the exponential mixing model, we can estimate the error in the reported mole fraction of nitrogen (as proxy for diborane) by taking the difference between the measured concentrations and the exponential fits. Those residuals are shown below:

![Estimated errors in mole fractions vs. concentration of nitrogen](image)

**Conclusions**

The estimated rms error for the measurement of the concentration of nitrogen (or diborane) in hydrogen is about 0.036% over the entire range. The mole fraction error is less than 0.05% for concentrations below 20%. For the particular instrument used, the error happened to be smallest for low concentrations of nitrogen, however the user can null the error at either 0% or 100% concentration by using the “Rel” feature of the instrument.