Target Gas Density Calculator Concept, Usage & Limitations

NIF Users’ Forum

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Mac conversion by Curtis Walters, PhD

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Why Have a Gas Density Calculator?

- In 2012, it was realized that the non-ideality of subcritical THD gas mixtures exceeded the allowable uncertainty of the capsule density.
  - Why? Conversion from density to pressure was not accurate using the Ideal Gas Law alone.
  - Jim Fair authored the first calculator that calculated the density of the isotopic mixtures of hydrogen and helium.
  - Other gases & gas mixtures being shot are similarly non-ideal. E.g., Neopentane.

- Primary purpose
  - To calculate an accurate conversion of density (mg/cm\(^3\)) to pressure (torr) in target gas fill requests.
  - To quantify the non-ideal behavior of subcritical or high pressure gases and gas mixtures.

- Secondary purposes
  - To predict the equilibrium of THD mixtures (H\(_2\), D\(_2\), T\(_2\), HD, HT, DT) from cryogenic to room temperature.
  - To predict the atomic particle density (atoms/cm\(^3\)).
Model Approach To Non-Ideality Corrections

- Virial Coefficient Corrections to the Ideal Gas Law
  \[ z = \frac{P}{RT\rho_m} \approx 1 + B_0\rho_m + C_0\rho_m^2 + ... \]
  
  - Mixing Rules (generally accepted for B, but not universally accepted for C)
    - 2\text{nd} Virial Coefficient – for low pressure, low temp or moderate pressure, high temperature gases
      \[ B_{ij} = \frac{(B_i + B_j)}{2} \]
      \[ B_{mix} = \sum_{i=1}^{N} y_i B_{ii} + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \delta_{ij} \]
      \[ \delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \]
    - 3\text{rd} Virial Coefficient – for high pressure gases near critical temperature
      \[ C_{ijk} = \frac{(C_i + C_j + C_k)}{3} \]
      \[ C_{mix} = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} y_i y_j y_k C_{ijk} \]
Caveats

- How good are the predictions? As good as the data.
  - E.g., Vapor pressure. Sources include:
    - Correlations from NIST
    - Compilation of literature data – polynomial fit
    - Antoine equation
  - THD Virial Coefficients
    - 2\textsuperscript{nd} VC - High Confidence:
      - From PIMC models, which match historical data from Souers, Sherwood, Reed, Grilly and others, and is valid from 15K through RT.
    - 3\textsuperscript{rd} VC - Unproven:
      - Is estimated using H\(_2\) 3\textsuperscript{rd} VC data and a corresponding states mapping (about T\(_r\)) from the 2\textsuperscript{nd} VCs.

- Programming sanity checks is time consuming
  - Use your own judgment and knowledge of the materials being studied.
  - When in doubt, call me.
Using the Density Calculator (Demo)

- **V2.5 & above:**
  - On a PC: Open the document, accept that Macros need to be run.
  - Navigate to the “Calculator” tab.
  - Enter the desired mass density & shot temperature.
  - Adjust the composition.
  - Check the right hand fields.
  - Find the pressure alongside the desired composition

- **V2.4 (Mac)**
  - Open the document.
  - Navigate to the “Calculator” tab.
  - Enter the desired mass density & shot temperature.
  - Adjust the composition.
  - For THD Mixtures ONLY:
    - N.B. Click the “THD Mixture Calculate” button. Wait for convergence.
      - If there is no convergence, navigate to the “THD Equilibrium Calculator” tab
        - Click “Reset” and “Solve” buttons.
        - Adjust “initial value factor” if necessary.
        - Re-click “Solve” to increase the number of solver iterations.
  - Check the right hand fields.
  - Find the pressure alongside the desired composition

- **V2.6 beta**
  - Working to resolve the issue of porting VB from PC to Mac version.
Using the Density Calculator (Demo)

- Case 1: Recent D$_2$-Filled HDC Symcap shot (N151025-001)
- Case 2: How do I request a specific density/mixture?
- Case 3: Post shot re-verification
Using the Density Calculator – Case 1

- Recent D₂-Filled HDC Symcap shot (N151025-001)
  - Original desired density:
    - 4 mg/cc at 32K
  - AppMan Request
    - 1486 Torr at 24K
  - Fielded Capsule
    - Liquid Deuterium
  - What red flags existed?
Using the Density Calculator (Case 2)

- Case 2: How do I request a specific density/mixture?
  - 10 mg/cc of D$_2$ at 32K
    • Answer should be immediately available
  - 10 mg/cc of 0.4 at% D$^3$He at 32K
  - 10 mg/cc of 50:50 DT at 32K
    • Mac: must click solver button
  - 10 mg/cc of 2/24/74 HDT at 32K
    • Mac: must click solver button
Using the Density Calculator (Demo)

- Case 3: Post shot analysis
  - Requested: 10 mg/cc of 0.75/0.25 HT at 32K
    • Calculator indicates: 5022 Torr at 32K.

  - Cryo Reports on !DATA:
    • 5069 Torr
    • Mass Spec Analysis
      - 74% H
      - 25% T
      - 1% D

    • Calculator (trial & error)
      - 10.21 mg/cc at 32K

  - NOTE: 75/25 from calculator is 10.13 mg/cc
Current ELM Version is NIF-0135638-AF or v2.5

- Recently added/changed features
  - On the PC version, the THD Equilibrium Calculator is now “live,” no need to hit a reset & run-macro button
    - Seems to work for three-component THD mixtures.
    - Uses a pragmatic “forced-mass-balance” scheme to converge the equilibrium expressions.
  - Science fiction checks
    - Polynomial correlation of saturated vapor density of THD.
    - Color coding: an indication of when an estimate is violating something
      - **Green** is good
      - **Red** is bad
      - Any other color: **Use with Caution**
        - Data may be extrapolated or near some critical value (e.g., saturation temp, valid range of vapor pressure expression, etc.)

- If its broken, or if the calculator doesn’t have a mixture or material that is of interest, contact me.