Target Gas Density Calculator Concept, Usage & Limitations

NIF Users' Forum

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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
  - $z = \frac{P}{RT\rho_m} \approx 1 + B\rho_m + C{\rho_m}^2 + \ldots$
  - Mixing Rules (generally accepted for B, but not universally accepted for C)
    - 2nd Virial Coefficient – for low pressure, low temp or moderate pressure, high temperature gases
      - $B_{ij} = \frac{(B_i + B_j)}{2}$
      - $B_{mix} = \sum_{i=1}^{N} y_i B_{ii} + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \delta_{ij}$
      - $\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj}$
    - 3rd 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^{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^{rd} VC - Unproven:
      - Is estimated using H_2 3^{rd} VC data and a corresponding states mapping (about T_r) from the 2^{nd} VCs.

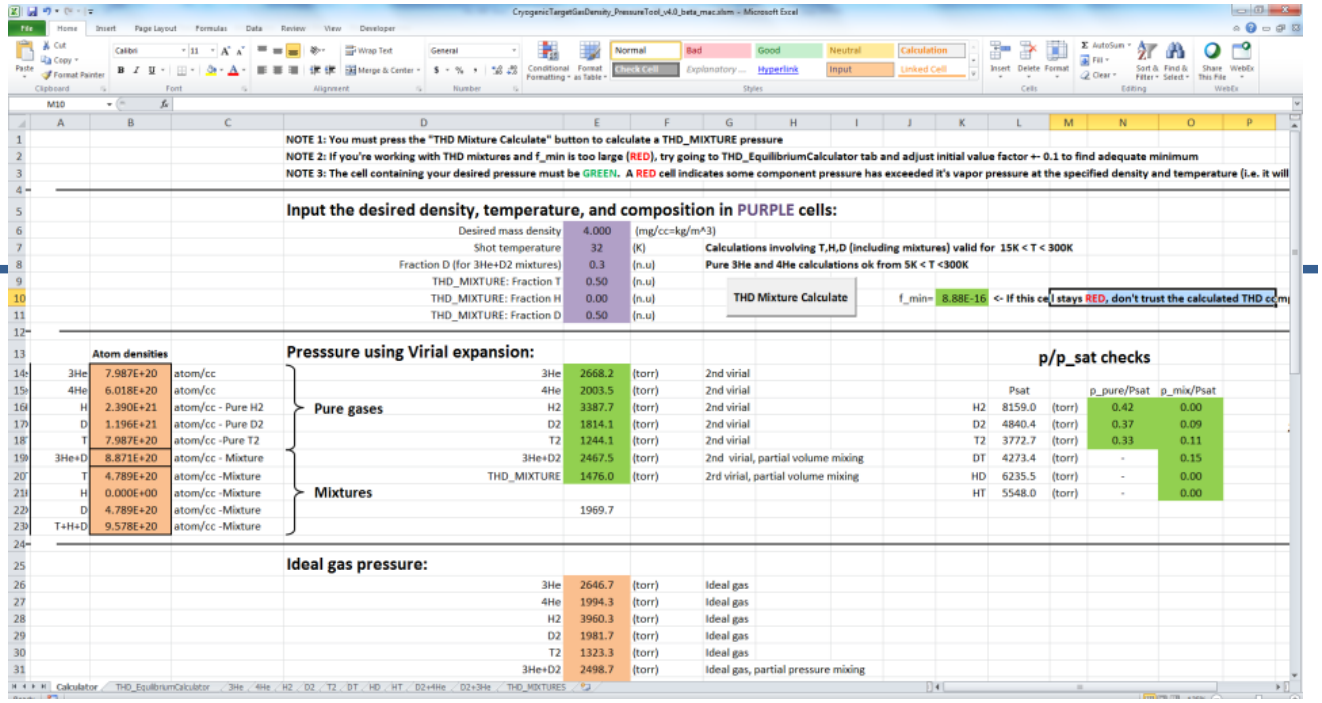
- Programming sanity checks is time consuming
  - Use your own judgment and knowledge of the materials being studied.
  - When in doubt, call me.

Using the Density Calculator (Demo)

- Case 1: 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

- D_2-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?



NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m^3)	
Shot temperature	32	(K)	Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)	Pure 3He and 4He calculations ok from 5K < T <300K
THD_MIXTURE: Fraction T	0.50	(n.u)	
THD_MIXTURE: Fraction H	0.00	(n.u)	THD Mixture Calculate
THD_MIXTURE: Fraction D	0.50	(n.u)	

f_min= 8.88E-16 <- If this cell stays RED, don't trust the calculated THD co

Atom densities		
3He	7.987E+20	atom/cc
4He	6.018E+20	atom/cc
H	2.390E+21	atom/cc - Pure H2
D	1.196E+21	atom/cc - Pure D2
T	7.987E+20	atom/cc -Pure T2
3He+D	8.871E+20	atom/cc - Mixture
T	4.789E+20	atom/cc -Mixture
H	0.000E+00	atom/cc -Mixture
D	4.789E+20	atom/cc -Mixture
T+H+D	9.578E+20	atom/cc -Mixture

Presssure using Virial expansion:

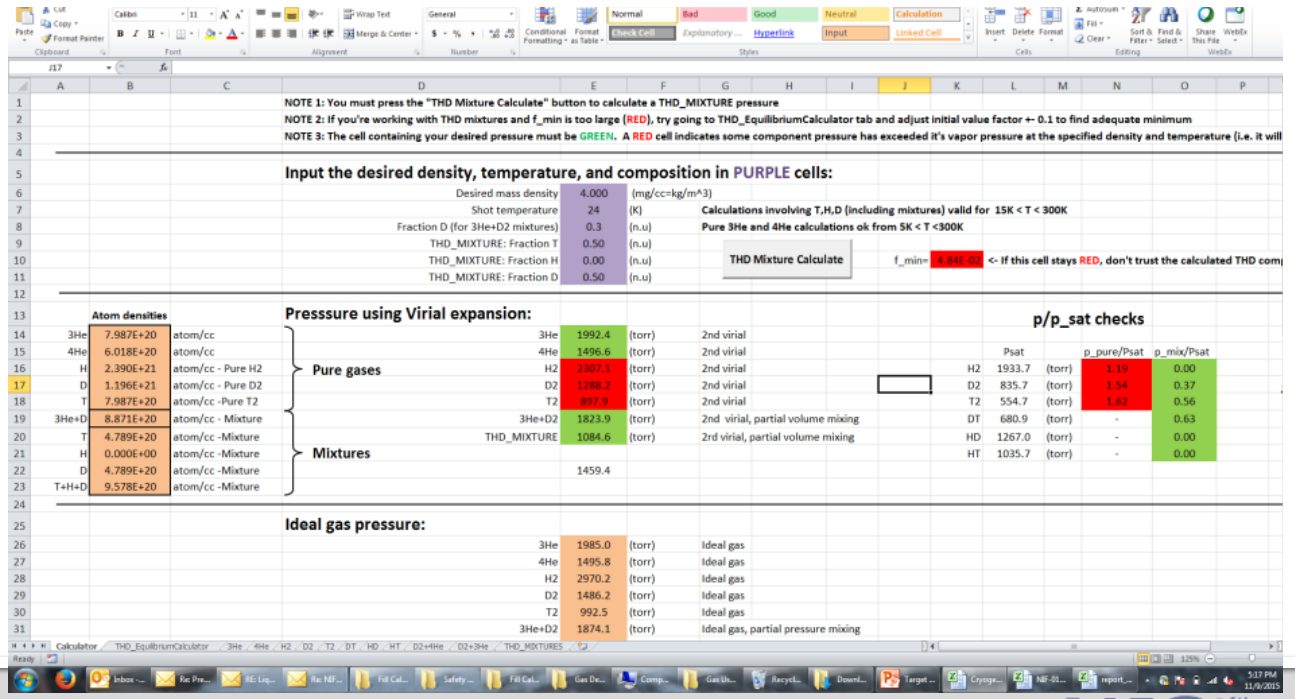
Pure gases	3He	2668.2	(torr)	2nd virial	
	4He	2003.5	(torr)	2nd virial	
	H2	3387.7	(torr)	2nd virial	
	D2	1814.1	(torr)	2nd virial	
	T2	1244.1	(torr)	2nd virial	
Mixtures	3He+D2	2467.5	(torr)	2nd virial, partial volume mixing	
	THD_MIXTURE	1476.0	(torr)	2rd virial, partial volume mixing	
		1969.7			

p/p_sat checks

	Psat		p_pure/Psat	p_mix/Psat
H2	8159.0	(torr)	0.42	0.00
D2	4840.4	(torr)	0.37	0.09
T2	3772.7	(torr)	0.33	0.11
DT	4273.4	(torr)	-	0.15
HD	6235.5	(torr)	-	0.00
HT	5548.0	(torr)	-	0.00

Ideal gas pressure:

3He	2646.7	(torr)	Ideal gas
4He	1994.3	(torr)	Ideal gas
H2	3960.3	(torr)	Ideal gas
D2	1981.7	(torr)	Ideal gas
T2	1323.3	(torr)	Ideal gas
3He+D2	2498.7	(torr)	Ideal gas, partial pressure mixing



NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m^3)	
Shot temperature	24	(K)	Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)	Pure 3He and 4He calculations ok from 5K < T <300K
THD_MIXTURE: Fraction T	0.50	(n.u)	
THD_MIXTURE: Fraction H	0.00	(n.u)	THD Mixture Calculate
THD_MIXTURE: Fraction D	0.50	(n.u)	

f_min= 4.84E-02 <- If this cell stays RED, don't trust the calculated THD com

Atom densities		
3He	7.987E+20	atom/cc
4He	6.018E+20	atom/cc
H	2.390E+21	atom/cc - Pure H2
D	1.196E+21	atom/cc - Pure D2
T	7.987E+20	atom/cc -Pure T2
3He+D	8.871E+20	atom/cc - Mixture
T	4.789E+20	atom/cc -Mixture
H	0.000E+00	atom/cc -Mixture
D	4.789E+20	atom/cc -Mixture
T+H+D	9.578E+20	atom/cc -Mixture

Presssure using Virial expansion:

Pure gases	3He	1992.4	(torr)	2nd virial	
	4He	1496.6	(torr)	2nd virial	
	H2	2307.1	(torr)	2nd virial	
	D2	1288.2	(torr)	2nd virial	
	T2	897.9	(torr)	2nd virial	
Mixtures	3He+D2	1823.9	(torr)	2nd virial, partial volume mixing	
	THD_MIXTURE	1084.6	(torr)	2rd virial, partial volume mixing	
		1459.4			

p/p_sat checks

	Psat		p_pure/Psat	p_mix/Psat
H2	1933.7	(torr)	1.19	0.00
D2	835.7	(torr)	1.54	0.37
T2	554.7	(torr)	1.62	0.56
DT	680.9	(torr)	-	0.63
HD	1267.0	(torr)	-	0.00
HT	1035.7	(torr)	-	0.00

Ideal gas pressure:

3He	1985.0	(torr)	Ideal gas
4He	1495.8	(torr)	Ideal gas
H2	2970.2	(torr)	Ideal gas
D2	1486.2	(torr)	Ideal gas
T2	992.5	(torr)	Ideal gas
3He+D2	1874.1	(torr)	Ideal gas, partial pressure mixing

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-AJ or v2.8

- 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.