Abundance variables first derivatives - 12Aug2017

The composition derivatives are perhaps more nuanced than one might initially imagine because one of them is special.

Baryon number is an invariant. Define the abundance of species Y_i by

$$Y_i = \frac{n_i}{n_B} = \frac{N_i}{N_B} \tag{1}$$

where N_i is the number of particles of isotope i, N_B is the number of baryons, n_i is the number density [cm^{-3}] of isotope i and n_B is baryon number density [cm^{-3}]. Define the average of any quantity $\overline{\beta}$ by the number density n_i weighted average

$$\overline{\beta} = \frac{\sum \beta_i n_i}{\sum n_i} \tag{2}$$

with equation (1) becomes

$$\overline{\beta} = \frac{\sum \beta_i Y_i}{\sum Y_i} \; . \tag{3}$$

The partial derivative with respect to abundance Y_i is

$$\frac{\partial \overline{\beta}}{\partial Y_i} = \frac{\beta_i}{\sum Y_i} - \frac{\sum \beta_i Y_i}{(\sum Y_i)^2} = \frac{\beta_i}{\sum Y_i} - \frac{\overline{\beta}}{\sum Y_i} = \frac{\beta_i - \overline{\beta}}{\sum Y_i} \; . \tag{4}$$

In this case,

$$\begin{aligned} \frac{\partial \overline{\mathrm{A}}}{\partial Y_i} &= \frac{A_i - \overline{\mathrm{A}}}{\sum Y_i} \\ \frac{\partial \overline{\mathrm{Z}}}{\partial Y_i} &= \frac{Z_i - \overline{\mathrm{Z}}}{\sum Y_i} \end{aligned} \tag{5}$$

However, reconsider the special case when the arbitrary quantity β_i is the number of nucleons A_i. As shown earlier, baryon conservation requires $\sum X_i = \sum A_i Y_i = n_B/n_B = 1$. Then $\overline{\mathrm{A}} = 1/\sum Y_i$ and another valid expression for $\partial \overline{\mathrm{A}}/\partial Y_i$ is

$$\begin{aligned} \frac{\partial \overline{\mathrm{A}}}{\partial Y_i} &= -\overline{\mathrm{A}}^2 \\ \frac{\partial \overline{\mathrm{Z}}}{\partial Y_i} &= \overline{\mathrm{A}} \, (Z_i - \overline{\mathrm{Z}}) \; . \end{aligned} \tag{6}$$

Despite looking very different, equations (5) and (6) are equivalent, provided one consistently uses either set of expressions. Mixing the two formalisms, essentially when to set $\sum X_i = 1$, causes confusion and incorrect results. Let's show the equivalence for the two forms of $d\overline{\mathrm{A}}/dY_i$.

The ideal gas

$$P = \left(\sum n_i\right) kT \ = \ \left(\sum Y_i\right) n_B kT \ , \tag{7}$$

has the trivial first derivative with respect to abundance

$$\frac{\partial P}{\partial Y_i} = n_B kT \tag{8}$$

Consider the formalism of equation (5) where $\sum X_i = 1$ was not explicitly invoked. The ideal gas law, using equation (5) becomes

$$P = n_B kT \left(\sum Y_i\right) \ = \ n_B kT \left(\frac{\sum \mathrm{A}_i Y_i}{\overline{\mathrm{A}}}\right) \ . \tag{9}$$

The derivative with respect to abundance is

$$\begin{aligned}
\frac{\partial P}{\partial Y_i} \ &= \ n_B kT \left[\frac{\mathrm{A}_i}{\overline{\mathrm{A}}} - \frac{\sum \mathrm{A}_i Y_i}{\overline{\mathrm{A}}^2} \ \frac{\partial \overline{\mathrm{A}}}{\partial Y_i}\right] \\
&= \ n_B kT \left[\frac{\mathrm{A}_i}{\overline{\mathrm{A}}} - \frac{\sum \mathrm{A}_i Y_i}{\overline{\mathrm{A}}^2} \ \left(\frac{\mathrm{A}_i - \overline{\mathrm{A}}}{\sum Y_i}\right)\right] \\
&= \ n_B kT \left[\frac{\mathrm{A}_i}{\overline{\mathrm{A}}} - \frac{\mathrm{A}_i}{\overline{\mathrm{A}}^2} \frac{\sum \mathrm{A}_i Y_i}{\sum Y_i} + \frac{1}{\overline{\mathrm{A}}} \frac{\sum \mathrm{A}_i Y_i}{\sum Y_i}\right] \\
&= \ n_B kT \left[\frac{\mathrm{A}_i}{\overline{\mathrm{A}}} - \frac{\mathrm{A}_i}{\overline{\mathrm{A}}} + 1\right] \\
&= \ n_B kT
\end{aligned} \tag{10}$$

which is identical to equation (8).

Consider the formalism of equation (6) where $\sum X_i = 1$ is used. The ideal gas law becomes

$$P = n_B kT \left(\sum Y_i\right) \ = \ \frac{n_B kT}{\overline{\mathrm{A}}} \ . \tag{11}$$

The derivative with respect to abundance is

$$\frac{\partial P}{\partial Y_i} \ = \ \frac{\partial P}{\partial \overline{\mathrm{A}}} \frac{\partial \overline{\mathrm{A}}}{\partial Y_i} \ = \ \left[-\frac{n_B kT}{\overline{\mathrm{A}}^2}\right]\left[-\overline{\mathrm{A}}^2\right] \ = \ n_B kT \tag{12}$$

which is identical to equation (8).

This shows either formalism may be used, provided it is used consistently. Since many expressions that use $\overline{\mathrm{A}}$ are written in the form of equation (11) rather than equation (9), the first derivative form of equation (6) is preferred.