Abundance variables first derivative examples - 12Aug2017

We've previously shown the mean atomic number

$$\overline{\mathrm{A}} = \frac{\sum n_i \mathrm{A}_i}{\sum n_i} = \frac{\sum Y_i \mathrm{A}_i}{\sum Y_i} = \frac{1}{\sum Y_i} \tag{1}$$

and mean charge

$$\overline{\mathrm{Z}} = \frac{\sum n_i \mathrm{Z}_i}{\sum n_i} = \frac{\sum Y_i \mathrm{Z}_i}{\sum Y_i} = \overline{\mathrm{A}} \sum Y_i \mathrm{Z}_i \tag{2}$$

have derivatives

$$\frac{d\overline{\mathrm{A}}}{dY_i} = -\overline{\mathrm{A}}^2 \tag{3}$$

and

$$\frac{\partial \overline{\mathrm{Z}}}{\partial Y_i} = \overline{\mathrm{A}}\,(\mathrm{Z}_i - \overline{\mathrm{Z}}) \tag{4}$$

respectively. For an arbitrary quantity β that is written in terms of $\overline{\mathrm{A}}$ and $\overline{\mathrm{Z}}$, the derivative with respect to Y_i is

$$\frac{d\beta}{dY_i} = \frac{\partial \beta}{\partial \overline{\mathrm{Z}}} \frac{\partial \overline{\mathrm{Z}}}{\partial Y_i} + \frac{\partial \beta}{\partial \overline{\mathrm{A}}} \frac{\partial \overline{\mathrm{A}}}{\partial Y_i} = \frac{\partial \beta}{\partial \overline{\mathrm{Z}}}\,\overline{\mathrm{A}}\,(\mathrm{Z}_i - \overline{\mathrm{Z}}) - \frac{\partial \beta}{\partial \overline{\mathrm{A}}}\,\overline{\mathrm{A}}^2 . \tag{5}$$

One assumes all partials of β with respect to $\overline{\mathrm{A}}$ and $\overline{\mathrm{Z}}$ are available from the physics is at hand (e.g., from an eos).

One simple but relevant example is the specific energy of an ideal gas

$$e = \frac{3}{2}\frac{P}{\rho} = \frac{3}{2}\frac{N_A kT}{\overline{\mathrm{A}}} \quad \mathrm{erg\ g^{-1}} \tag{6}$$

has the partial derivative of with respect to $\overline{\mathrm{Z}}$

$$\frac{\partial e}{\partial \overline{\mathrm{Z}}} = 0 \tag{7}$$

and the partial derivative of with respect to $\overline{\mathrm{A}}$

$$\frac{\partial e}{\partial \overline{\mathrm{A}}} = -\frac{3}{2}\frac{N_A kT}{\overline{\mathrm{A}}^2} . \tag{8}$$

Hence by equation (5) the derivative with respect to Y_i is

$$\frac{de}{dY_i} = \frac{\partial e}{\partial \overline{\mathrm{Z}}} \frac{\partial \overline{\mathrm{Z}}}{\partial Y_i} + \frac{\partial e}{\partial \overline{\mathrm{A}}} \frac{\partial \overline{\mathrm{A}}}{\partial Y_i} = \left[-\frac{3}{2}\frac{N_A kT}{\overline{\mathrm{A}}^2} \right] \left[-\overline{\mathrm{A}}^2 \right] = \frac{3}{2} N_A kT \quad \mathrm{erg\ g^{-1}} \tag{9}$$

as expected when recasting equation (6) as

$$e = \frac{3}{2}\frac{P}{\rho_B} = \frac{3}{2}\, N_A kT \sum Y_i \quad \mathrm{erg\ g^{-1}} . \tag{10}$$

Note $\partial e / \partial Y_i$ is usually known as the chemical potential in the first law of thermodynamics when composition changes are taken into account.

Another example is the mean molecular weight

$$\mu = \left[\frac{1}{\mu_{ion}} + \frac{1}{\mu_{ele}}\right]^{-1} = \left[\frac{1}{\overline{\mathrm{A}}} + Y_e\right]^{-1} = \left[\frac{1}{\overline{\mathrm{A}}} + \frac{\overline{\mathrm{Z}}}{\overline{\mathrm{A}}}\right]^{-1} = \frac{\overline{\mathrm{A}}}{\overline{\mathrm{Z}} + 1} = \frac{n_B}{\sum n_i + n_e} \ . \tag{11}$$

The partial derivative of μ with respect to $\overline{\mathrm{Z}}$ is

$$\frac{\partial\mu}{\partial\overline{\mathrm{Z}}} = \frac{\partial}{\partial\overline{\mathrm{Z}}}\left(\frac{\overline{\mathrm{A}}}{\overline{\mathrm{Z}} + 1}\right) = -\frac{\overline{\mathrm{A}}}{\left(\overline{\mathrm{Z}} + 1\right)^2} = -\frac{\mu}{\overline{\mathrm{Z}} + 1} = -\frac{\mu^2}{\overline{\mathrm{A}}} \ . \tag{12}$$

The partial derivative of μ with respect to $\overline{\mathrm{A}}$ is

$$\frac{\partial\mu}{\partial\overline{\mathrm{A}}} = \frac{\partial}{\partial\overline{\mathrm{A}}}\left(\frac{\overline{\mathrm{A}}}{\overline{\mathrm{Z}} + 1}\right) = \frac{1}{\left(\overline{\mathrm{Z}} + 1\right)} = \frac{\mu}{\overline{\mathrm{A}}} \tag{13}$$

Applying equation (5), the derivative of μ with respect to Y_i is

$$\begin{aligned} \frac{d\mu}{dY_i} &= \frac{\partial\mu}{\partial\overline{\mathrm{Z}}}\frac{\partial\overline{\mathrm{Z}}}{\partial Y_i} + \frac{\partial\mu}{\partial\overline{\mathrm{A}}}\frac{\partial\overline{\mathrm{A}}}{\partial Y_i} = \left[-\frac{\mu^2}{\overline{\mathrm{A}}}\right]\left[\overline{\mathrm{A}}(\mathrm{Z}_i - \overline{\mathrm{Z}})\right] + \left[\frac{\mu}{\overline{\mathrm{A}}}\right]\left[-\overline{\mathrm{A}}^2\right] \\ &= \mu^2(\overline{\mathrm{Z}} - Z_i) - \mu\overline{\mathrm{A}} \end{aligned} \tag{14}$$

Sometimes the composition is defined in terms of the hydrogen baryon (mass) fraction $\mathcal{X}$, helium baryon (mass) $\mathcal{Y}$, and metal baryon (mass) $\mathcal{Z}$. Bayron number conservation is then expressed as

$$\mathcal{X} + \mathcal{Y} + \mathcal{Z} = 1 \ . \tag{15}$$

These abundance variables are related to the usual $Y_i = X_i\, A_i$ abundance variables by

$$\mathcal{X} = Y_{\mathrm{H}} \qquad \mathcal{Y} = 4Y_{\mathrm{He}} \qquad \mathcal{Z} = A_{\mathrm{z}} Y_{\mathrm{Z}} \ , \tag{16}$$

which mostly explains the use of calligraphic font to avoid the same symbols for different quantities. Applying equation (1)

$$\overline{\mathrm{A}} = \frac{1}{\mathcal{X} + \mathcal{Y}/4 + \mathcal{Z}/\mathrm{A_z}} = \frac{4A_{\mathrm{z}}}{\mathrm{A_z}\mathcal{X} + A_{\mathrm{z}}\mathcal{Y} + 4\mathcal{Z}} = \frac{4A_{\mathrm{z}}}{A_{\mathrm{z}} + 3A_{\mathrm{z}}\mathcal{X} + 4\mathcal{Z} - A_{\mathrm{z}}\mathcal{Z}} \ , \tag{17}$$

where the last expression eliminated $\mathcal{Y}$ using equation (15). Applying equation (2)

$$\begin{aligned} \overline{\mathrm{Z}} &= \frac{\mathcal{X} + 1/2\mathcal{Y} + \mathrm{Z_z}/\mathrm{A_z}\mathcal{Z}}{\mathcal{X} + \mathcal{Y}/4 + \mathcal{Z}/\mathrm{A_z}} \\ &= (\mathcal{X} + 1/2\mathcal{Y} + \mathrm{Z_z}/\mathrm{A_z}\mathcal{Z}) \cdot \overline{\mathrm{A}} \\ &= \frac{2A_{\mathrm{z}}(1 + \mathcal{X} - \mathcal{Z}) + 4Z_{\mathrm{z}}\mathcal{Z}}{A_{\mathrm{z}} + 3A_{\mathrm{z}}\mathcal{X} + 4\mathcal{Z} - A_{\mathrm{z}}\mathcal{Z}} \ , \end{aligned} \tag{18}$$

where again $\mathcal{Y}$ was eliminated using equation (15).

Then the first derivatives of $\overline{\mathrm{A}}$ are

$$\frac{\partial\overline{\mathrm{A}}}{\partial\mathcal{X}} = -\frac{12A_z^2}{(A_z + 3A_z\mathcal{X} + 4\mathcal{Z} - A_z\mathcal{Z})^2}$$

$$\frac{\partial\overline{\mathrm{A}}}{\partial\mathcal{Z}} = \frac{4A_z^2 - 16A_z}{(A_z + 3A_z\mathcal{X} + 4\mathcal{Z} - A_z\mathcal{Z})^2} \qquad (19)$$

The first derivatives of $\overline{\mathrm{Z}}$ are

$$\frac{\partial\overline{\mathrm{Z}}}{\partial\mathcal{X}} = \frac{4A_z[A_z(\mathcal{Z} - 1) + \mathcal{Z}(2 - 3Z_z)]}{(A_z + 3A_z\mathcal{X} + 4\mathcal{Z} - A_z\mathcal{Z})^2}$$

$$\frac{\partial\overline{\mathrm{Z}}}{\partial\mathcal{Z}} = -\frac{4A_z[2 + \mathcal{X}(2(A_z - 3Z_z) - Z_z]}{(A_z + 3A_z\mathcal{X} + 4\mathcal{Z} - A_z\mathcal{Z})^2} \qquad (20)$$

For an arbitrary quantity β that is written in terms of $\overline{\mathrm{A}}$ and $\overline{\mathrm{Z}}$, the derivatives with respect to $\mathcal{X}$ and $\mathcal{Z}$ are

$$\frac{d\beta}{d\mathcal{X}} = \frac{\partial\beta}{\partial\overline{\mathrm{Z}}}\frac{\partial\overline{\mathrm{Z}}}{\partial\mathcal{X}} + \frac{\partial\beta}{\partial\overline{\mathrm{A}}}\frac{\partial\overline{\mathrm{A}}}{\partial\mathcal{X}}$$

$$\frac{d\beta}{d\mathcal{Z}} = \frac{\partial\beta}{\partial\overline{\mathrm{Z}}}\frac{\partial\overline{\mathrm{Z}}}{\partial\mathcal{Z}} + \frac{\partial\beta}{\partial\overline{\mathrm{A}}}\frac{\partial\overline{\mathrm{A}}}{\partial\mathcal{Z}} \qquad (21)$$

Note that equations (17) and (18) can be solved for the either unknown or inconvenient variables A_z and Z_z:

$$A_z = \frac{4\overline{\mathrm{A}}\mathcal{Z}}{4 - \overline{\mathrm{A}} - 3\overline{\mathrm{A}}\mathcal{X} - \overline{\mathrm{A}}\mathcal{Z}}$$

$$Z_z = \frac{4\overline{\mathrm{Z}} - 2\overline{\mathrm{A}}(1 + \mathcal{X} - \mathcal{Z})}{4 - \overline{\mathrm{A}} - 3\overline{\mathrm{A}}\mathcal{X} - \overline{\mathrm{A}}\mathcal{Z}}\ . \qquad (22)$$

Eliminating A_z and Z_z from equation (19) gives

$$\frac{\partial\overline{\mathrm{A}}}{\partial X} = -\frac{3\overline{\mathrm{A}}^2}{4}$$

$$\frac{\partial\overline{\mathrm{A}}}{\partial Z} = \frac{\overline{\mathrm{A}}\,(\overline{\mathrm{A}} + 3\overline{\mathrm{A}}\mathcal{X} - 4)}{4\mathcal{Z}}\ . \qquad (23)$$

Eliminating A_z and Z_z from equation (20) gives

$$\frac{\partial\overline{\mathrm{Z}}}{\partial X} = \frac{\overline{\mathrm{A}}\,(2 - 3\overline{\mathrm{Z}})}{4}$$

$$\frac{\partial\overline{\mathrm{Z}}}{\partial Z} = \frac{\overline{\mathrm{A}}\,[\overline{\mathrm{Z}} + (3\overline{\mathrm{Z}} - 2)\mathcal{X} - 2]}{4\mathcal{Z}}\ . \qquad (24)$$

Equation (21) still holds.