Nuclear Energy Generation Expressions - 12Aug2017

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}]. The number of baryons in isotope i divided by the total number of baryons is the baryon fraction X_i,

$$X_i = Y_i\, A_i = \frac{n_i\, A_i}{n_B} \tag{2}$$

where A_i is the atomic mass number, the number of baryons in an isotope. Usually the baryon fraction is called the "mass fraction". Note

$$\sum X_i = \frac{n_B}{n_B} = 1 \tag{3}$$

is invariant under nuclear reactions. Define the baryon density, in atomic mass units, as

$$\rho_B = n_B\, m_u = \frac{n_B}{N_A} \quad \text{g cm}^{-3} \tag{4}$$

where m_u is the atomic mass unit [g] and N_A is the Avogadro number [g^{-1}] in a system of units where the atomic mass unit is *defined* as 1/12 mass of an unbound atom of ^{12}C is at rest and in its ground state.

The rest-mass energy is

$$E = -Mc^2 \quad \text{erg} \tag{5}$$

where M is the total baryonic mass [g]. The minus sign indicates that creating mass reduces the energy reservoir of a closed system. For M being composed of i isotopes

$$E = -\sum_{i=1}^{k} N_i\, m_i\, c^2 \quad \text{erg}\ . \tag{6}$$

Multiplying by the constant N_A/N_B and using equation (1) gives gives the specific nuclear energy of the baryons

$$\epsilon = -N_A c^2 \sum_{i=1}^{k} Y_i\, m_i \quad \text{erg g}^{-1}\ . \tag{7}$$

Taking the time derivative yields the specific nuclear energy generation rate

$$\dot{\epsilon} = -N_A c^2 \sum_{i=1}^{k} \dot{Y}_i\, m_i \quad \text{erg g}^{-1}\ \text{s}^{-1} \tag{8}$$

Note one only needs to evaluate, not integrate, the right-hand sides of the $\dot{Y}_i$ ODEs defining the nuclear reaction network to obtain the instantaneous $\dot{\epsilon}$. Nice.

The atomic mass m_i in equation (8) can be defined as

$$m_i = \mathrm{A}_i m_u + \Delta_i \quad \mathrm{g} \tag{9}$$

where Δ_i is the mass excess of each species in atomic mass units [g]. This expression neglects the electronic binding energy, and Δ_i is thus independent of the ionization state of a given species. However, the electron rest masses are included in this definition since the m_i are atomic masses - this is important for accurately tracking weak reactions. The mass excess is related to the binding energy B_i, mass excess of the proton Δ_p and mass excess of the neutron Δ_n by

$$\Delta_i = \mathrm{Z}_i \Delta_p + N_i \Delta_n - \frac{B_i}{c^2} \quad \mathrm{g} \tag{10}$$

Substituting equations (9) and (10) into equation (8) gives

$$\dot{\epsilon} = -N_A c^2 \sum_{i=1}^{k} \dot{Y}_i \left(A_i m_u + \mathrm{Z}_i \Delta_p + N_i \Delta_n - \frac{B_i}{c^2} \right) \quad \mathrm{erg\ g^{-1}\ s^{-1}} \tag{11}$$

From equation (3), $\sum \dot{X}_i = \sum \dot{Y}_i \mathrm{A}_i = 0$, hence the above reduces to

$$\dot{\epsilon} = N_A \sum_{i=1}^{k} \dot{Y}_i B_i - \sum_{i=1}^{k} \dot{Y}_i (\mathrm{Z}_i \Delta_p + N_i \Delta_n) \quad \mathrm{erg\ g^{-1}\ s^{-1}} \tag{12}$$

This is a handy form as changes due to weak reactions are isolated by the second term on the right-hand side. If weak reactions are not important,

$$\dot{\epsilon} = N_A \sum_{i=1}^{k} \dot{Y}_i B_i \quad \mathrm{erg\ g^{-1}\ s^{-1}} \tag{13}$$

Equation (8) is the *instantaneous* energy generation rate. In this form it can be added as an ODE to the nuclear reaction network equations, or added to the system of PDEs in a fully coupled hydrocode. In an operator-split hydrocode, over a timestep Δt one usually uses the finite difference approximation

$$\dot{Y}_i = \frac{Y_{i,\mathrm{end}} - Y_{i,\mathrm{start}}}{\Delta t} \quad \mathrm{s^{-1}} \tag{14}$$

and equation (8) becomes

$$\langle \dot{\epsilon} \rangle = -N_A c^2 \sum_{i=1}^{k} \left[\frac{Y_{i,\mathrm{end}} - Y_{i,\mathrm{start}}}{\Delta t} \right] m_i \quad \mathrm{erg\ g^{-1}\ s^{-1}} \ , \tag{15}$$

and represents the average energy generation rate over a finite timestep.

A note on the mass of isotope i. The intuitive mass counting of nucleons minus the binding energy is

$$m_i = Z_i m_p + N_i m_n - \frac{B_i}{c^2} \qquad \mathrm{g} \tag{16}$$

Eliminating the binding energy B_i using equation (10)

$$\begin{aligned} m_i &= Z_i m_p + N_i m_n - \Delta_i - Z_i \Delta_p - N_i \Delta_m \\ &= Z_i(m_p - \Delta_p) + N_i(m_n - \Delta_n) - \Delta_i \end{aligned} \tag{17}$$

By definition, $m_p = m_u + \Delta_p \simeq (1 + 0.007276) m_u$ and $m_n = m_u + \Delta_n \simeq (1 + .008664) m_u$. Substituting,

$$\begin{aligned} m_i &= Z_i m_u + N_i m_u - \Delta_i \\ &= (Z_i + N_i) m_u - \Delta_i \\ &= A_i m_u - \Delta_i \end{aligned} \tag{18}$$

which is equation (9) for the atomic mass.