

Self-Heating - 12Aug2017

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

$$Y_i = \frac{n_i}{n_B} = \frac{N_i}{N_B} \quad (1)$$

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 ,

$$X_i = Y_i A_i = \frac{n_i A_i}{n_B} \quad (2)$$

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

$$\sum X_i = \frac{n_B}{n_B} = 1 \quad (3)$$

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

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

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 first law of thermodynamics is

$$dE = \delta Q - \delta W = \delta Q - PdV \quad \text{erg} \quad (5)$$

where dE is the change in internal energy and δQ is the heat added to the system. $\delta W = PdV$ is the mechanical work performed in expanding or contracting the system, where P [erg cm^{-3}] is the pressure and dV is the change in volume [cm^3].

If one *chooses* the entropy S [erg/K], volume V , and N_i as the independent thermodynamic variables, then the total differential of the internal energy is

$$\begin{aligned} dE &= \left(\frac{\partial E}{\partial S} \right)_{V, N_i} dS + \left(\frac{\partial E}{\partial V} \right)_{S, N_i} dV + \sum_i \left(\frac{\partial E}{\partial N_i} \right)_{S, V} dN_i \\ &= T dS - PdV + \sum_i \left(\frac{\partial E}{\partial N_i} \right)_{S, V} dN_i . \end{aligned} \quad (6)$$

Comparing equations (5) and (6), gives the familiar equality

$$\delta Q \equiv dE + PdV = T dS + \sum_i \left(\frac{\partial E}{\partial N_i} \right)_{S, V} dN_i \quad (7)$$

On the other hand, one may *choose* the temperature T , volume V , and N_i as the independent thermodynamic variables. Then the total differential of the internal energy is

$$\begin{aligned} dE &= \left(\frac{\partial E}{\partial T}\right)_{V,N_i} dT + \left(\frac{\partial E}{\partial V}\right)_{T,N_i} dV + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{T,V} dN_i \\ &= C_v dT - PdV + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{T,V} dN_i, \end{aligned} \quad (8)$$

where C_v is the specific heat [erg/K] at constant volume. Comparing equations (5) and (8) gives the following equality

$$\delta Q \equiv dE + PdV = TdS + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{S,V} dN_i = c_v dT + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{T,V} dN_i \quad (9)$$

Note the $\partial E/\partial N_i$ terms are sometimes called the chemical potential μ_i . The heat added to the system from nuclear reactions is

$$\delta Q = E_{\text{nuc}} - E_v \quad (10)$$

which gives the equalities

$$\begin{aligned} \delta Q &\equiv dE + PdV \\ &= TdS + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{S,V} dN_i \\ &= C_v dT + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{T,V} dN_i \\ &= E_{\text{nuc}} - E_v \end{aligned} \quad (11)$$

Multiplying by the constant N_A/N_B [1/g] gives the specific form of the first law:

$$\begin{aligned} \delta q &\equiv de + Pd\left(\frac{1}{\rho}\right) \\ &= Tds + \sum_i \left(\frac{\partial e}{\partial Y_i}\right)_{S,\rho} dY_i \\ &= c_v dT + \sum_i \left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} dY_i \\ &= \epsilon_{\text{nuc}} - \epsilon_v \quad \text{erg g}^{-1} \end{aligned} \quad (12)$$

Which could have been gotten by using the (T, ρ, Y_i) Helmholtz free energy triplet as the independent variables. Operating with the time derivative d/dt gives

$$\begin{aligned} \frac{de}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} &= T \frac{ds}{dt} + \sum_i \left(\frac{\partial e}{\partial Y_i}\right)_{S,\rho} \frac{dY_i}{dt} \\ &= c_v \frac{dT}{dt} + \sum_i \left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} \frac{dY_i}{dt} \\ &= \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v \quad \text{erg g}^{-1} \text{ s}^{-1} \end{aligned} \quad (13)$$

One may solve any combination of the expressions in equation (13).

It is interesting to consider equation (13) for an idea gas. It has been shown previously that the specific internal energy

$$e = \frac{3P}{2\rho} = \frac{3}{2} \frac{N_A k T}{A} = \frac{3}{2} N_A k T \sum_i Y_i \quad \text{erg g}^{-1} \quad (14)$$

has the derivative

$$\left(\frac{\partial e}{\partial Y_i} \right)_{\rho, N_{i \neq j}} = \frac{3}{2} N_A k T. \quad (15)$$

Its also been previously shown in these notes that nuclear energy generation rate is

$$\dot{\epsilon}_{\text{nuc}} = -N_A c^2 \sum_i \frac{dY_i}{dt} m_i \quad \text{erg g}^{-1} \text{ s}^{-1}. \quad (16)$$

Neglecting thermal neutrino losses, the temperature evolution version of equation (13) becomes

$$\begin{aligned} c_v \frac{dT}{dt} &= \dot{\epsilon}_{\text{nuc}} - \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T, \rho} \frac{dY_i}{dt} \\ &= -N_A c^2 \sum_i \frac{dY_i}{dt} m_i - \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T, \rho} \frac{dY_i}{dt} \\ &= -N_A c^2 \sum_i \frac{dY_i}{dt} m_i - \frac{3}{2} N_A k T \sum_i \frac{dY_i}{dt}. \end{aligned} \quad (17)$$

Physically equation (17) says the change in the energy is the energy release from nuclear reactions minus the thermal energy of the now heavier (and fewer) gas particles. For example, say there are 4 protons. Each has an energy of $3/2 kT$. When the 4 protons combine to form 1 helium nucleus, there is an energy gain from the nuclear reaction but now there is only 1 particle with an energy of $3/2 kT$. The system gains energy because

$$\frac{m_{4\text{He}} - 4m_p}{4m_p} \cdot c^2 \simeq 0.007 \cdot c^2 \simeq 0.007 \cdot 10^{21} \gg N_A k T \simeq 8 \times 10^{14} \cdot \left(\frac{T}{10^7 \text{K}} \right) \quad \text{erg g}^{-1}. \quad (18)$$

for typical hydrogen burning temperatures. At the other extreme, the system loses energy when the second term in equation (17) becomes larger than the first term. At temperatures of $\simeq 10^{10}$ K, this occurs when the relative mass change from nuclear burning becomes smaller than $\eta = \Delta m/m = N_A k T / c^2 \simeq 8 \times 10^{16} / 10^{21} \simeq 10^{-4}$, about a factor of 100 smaller than hydrogen burning's 0.007. In general, when

$$\frac{N_A k T}{\eta c^2} \ll 1 \quad (19)$$

the second term in equation (13) can be safely dropped.

Let's consider a few specific instantiations of equation (13).

For self-heating at constant density, $d\rho = 0$, and equation(13) reduces to

$$\frac{de}{dt} = c_v \frac{dT}{dt} + \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T,\rho} \frac{dY_i}{dt} = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v . \quad (20)$$

is a convenient form. If one evolves the specific energy, one must do a root find on the equation of state to get the temperature for a given (e, ρ, Y_i) triplet. If one evolves the temperature directly, the $\partial e/\partial Y_i$ terms must be included:

$$\frac{dT}{dt} = \frac{1}{c_v} \left[\dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T,\rho} \frac{dY_i}{dt} \right] \quad \text{K s}^{-1} . \quad (21)$$

For self-heating at constant pressure, one approach is to solve equation (21) and do a root find on the equation of state to get the density for a given (T, P, Y_i) triplet - a Gibbs free energy basis set. *This is the easiest approach.* Alternatively, the hard way, expanding the total specific energy differential of equation (13) in the (T, ρ, Y_i) Helmholtz free energy basis gives

$$\begin{aligned} \frac{de}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} &= \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v \\ \left(\frac{\partial e}{\partial T} \right)_{\rho, Y_i} \frac{dT}{dt} + \left(\frac{\partial e}{\partial \rho} \right)_{T, Y_i} \frac{d\rho}{dt} + \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T, \rho} \frac{dY_i}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} &= \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v \\ \left(\frac{\partial e}{\partial T} \right)_{\rho, Y_i} \frac{dT}{dt} + \left[\left(\frac{\partial e}{\partial \rho} \right)_{T, Y_i} - \frac{P}{\rho^2} \right] \frac{d\rho}{dt} &= \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T, \rho} \frac{dY_i}{dt} . \end{aligned} \quad (22)$$

Now, the first law is an exact differential, which requires

$$P = \rho^2 \left(\frac{\partial e}{\partial \rho} \right)_{T, Y_i} + T \left(\frac{\partial P}{\partial T} \right)_{\rho, Y_i} . \quad (23)$$

Using equation (23) to eliminate $(\partial e/\partial \rho)_{T, Y_i}$ in equation (22) gives

$$c_v \frac{dT}{dt} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_{\rho, Y_i} \frac{d\rho}{dt} = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left(\frac{\partial e}{\partial Y_i} \right)_{T, \rho} \frac{dY_i}{dt} . \quad (24)$$

In addition, for constant pressure, the total differential is $dP = 0$

$$dP = \left(\frac{\partial P}{\partial T} \right)_{\rho, Y_i} dT + \left(\frac{\partial P}{\partial \rho} \right)_{T, Y_i} d\rho + \sum_i \left(\frac{\partial P}{\partial Y_i} \right)_{T, \rho} dY_i = 0 . \quad (25)$$

Solving for $d\rho$,

$$d\rho = -\frac{1}{\left(\frac{\partial P}{\partial \rho}\right)_{T,Y_i}} \left[\left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} dT + \sum_i \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} dY_i \right]. \quad (26)$$

Substituting equation (26) into equation (24)

$$c_v \frac{dT}{dt} + \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \left[\left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} \frac{dT}{dt} + \sum_i \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} \frac{dY_i}{dt} \right] = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} \frac{dY_i}{dt} \quad (27)$$

Rearranging,

$$\left[c_v + \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i}^2 \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \right] \frac{dT}{dt} = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left[\left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} + \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} \right] \frac{dY_i}{dt} \quad (28)$$

using the so-called thermal and density exponents

$$\chi_t = \frac{T}{P} \frac{\partial P}{\partial T} \quad \chi_\rho = \frac{\rho}{P} \frac{\partial P}{\partial \rho} \quad (29)$$

one has

$$\left[c_v + \frac{P}{\rho T} \frac{\chi_t}{\chi_\rho} \right] \frac{dT}{dt} = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left[\left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} + \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} \right] \frac{dY_i}{dt} \quad (30)$$

or

$$c_p \frac{dT}{dt} = \dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left[\left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} + \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} \right] \frac{dY_i}{dt}, \quad (31)$$

where c_p [erg g⁻¹ K⁻¹] is the specific heat at constant pressure. Hence, the final temperature evolution equation for a fixed pressure and changing composition:

$$\frac{dT}{dt} = \frac{1}{c_p} \left[\dot{\epsilon}_{\text{nuc}} - \dot{\epsilon}_v - \sum_i \left[\left(\frac{\partial e}{\partial Y_i}\right)_{T,\rho} + \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_{\rho,Y_i} \left(\frac{\partial \rho}{\partial P}\right)_{T,Y_i} \left(\frac{\partial P}{\partial Y_i}\right)_{T,\rho} \right] \frac{dY_i}{dt} \right]. \quad (32)$$

Whew. Equation (21) with a root find is simpler.

For self-heating at entropy, a model for a burning convective region, one approach is to solve equation (21) and do a root find on the equation of state to get the density for a given (T, S, Y_i) triplet. Alternatively, the hard way, is to follow the example above to get an explicit evolution equation for the entropy.