Reaction Networks - 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 continuity equation for the number density of species i in an Eulerian framework is

$$\frac{\partial n_i}{\partial t} + \frac{\partial (n_i v_x)}{\partial x} = \sum_{j,k} r_{jk} n_j n_k \quad \text{cm}^{-3}\ \text{s}^{-1} \tag{5}$$

where the reaction rate between two species j and k is

$$r_{jk} = <\sigma v>_{jk} \quad \text{cm}^{3}\ \text{s}^{-1} \tag{6}$$

and $<\sigma v>_{jk}$ is the cross-section σ [in cm^2] times the relative speed v [in cm s^{-1}] between the two isotopes, and the angled brackets indicates an average over a statistical distribution, usually a Maxwell-Boltzmann. r_{jk} is a function of temperature only. The reaction rate implies a lifetime for isotope j of $\tau_j = 1/(n_j r_{jk})$ s.

Nuclear reactions, and expansion or contraction of the plasma can produce changes in the number densities n_i. To separate the nuclear changes in composition from hydrodynamic effects, substituting equation (1) gives

$$\frac{\partial(Y_i n_B)}{\partial t} + \frac{\partial(Y_i n_B v_x)}{\partial x} = \sum_{j,k} r_{j,k} Y_j Y_k n_B^2$$

$$n_B \frac{\partial Y_i}{\partial t} + Y_i \frac{\partial n_B}{\partial t} + n_B \frac{\partial(Y_i v_x)}{\partial x} + Y_i \frac{\partial(n_B v_x)}{\partial x} = \sum_{j,k} r_{j,k} Y_j Y_k n_B^2$$

$$n_B \left(\frac{\partial Y_i}{\partial t} + \frac{\partial(Y_i v_x)}{\partial x} \right) + Y_i \left[\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_x)}{\partial x} \right] = \sum_{j,k} r_{j,k} Y_j Y_k n_B^2 \tag{7}$$

The term in square brackets is zero by the mass continuity equation. Thus,

$$\frac{\partial Y_i}{\partial t} + \frac{\partial(Y_i v_x)}{\partial x} = \sum_{j,k} r_{j,k} n_B Y_j Y_k \quad \mathrm{s}^{-1} \tag{8}$$

or in a Lagrangian frame

$$\frac{dY_i}{dt} = \sum_{j,k} r_{j,k} n_B Y_j Y_k = \sum_{j,k} r_{j,k} N_A \rho Y_j Y_k \quad \mathrm{s}^{-1} \tag{9}$$

In an operator split Eularian hydrocode, the advection term is done seperately, leading to the same ordinary differential equations to solve as in the Lagrangian form.

Common reaction rate compilations list $\lambda = N_A < \sigma v >_{jk}$ [in cm^3 g^{-1} s^{-1}], so

$$\frac{dY_i}{dt} = \sum_{j,k} \lambda_{j,k} \rho Y_j Y_k \quad \mathrm{s}^{-1} \tag{10}$$

Let $R_{j,k} = \lambda_{j,k}\rho$ be the “reaction rate” that subsumes all the temperature and density dependences. Then,

$$\frac{dY_i}{dt} = \sum_{j,k} R_{j,k} Y_j Y_k \quad \mathrm{s}^{-1} \tag{11}$$

are the equations that constiture a nuclear reaction network.