Title: Equation-of-State Scaling Factors

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Intended for: LA-UR publication

Issued: 2016-06-28

Equation-of-State Scaling Factors

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June 10, 2016

Equation-of-State scaling factors are needed when using a tabular EOS in which the user defined material isotopic fractions differ from the actual isotopic fractions used by the table. Additionally, if a material is dynamically changing its isotopic structure, then an EOS scaling will again be needed, and will vary in time and location. The procedure that allows use of a table to obtain information about a similar material with average atomic mass M_s and average atomic number Z_s is described below. The procedure is exact for a fully ionized ideal gas. However, if the atomic number is replace by the effective ionization state the procedure can be applied to partially ionized material as well, which extends the applicability of the scaling approximation continuously from low to high temperatures.

Assume that a tabular EOS which is a function of density, ρ_t and specific internal energy ϵ_t is given as

$$P_t = P_t(\rho_t, \epsilon_t) \tag{1}$$

In addition, the table material has an an average atomic mass of M_t and and average atomic number of Z_t. For and ideal gas the pressure, energy density and specific internal energy are:

$$P_t = N(Z_t + 1)k_\beta T \tag{2}$$

$$E_t = N((Z_t + 1)/(\gamma_t - 1))k_\beta T \tag{3}$$

$$\epsilon_t = E_t/\rho_t = ((Z_t + 1)/(\gamma_t - 1))k_\beta T/M_t \tag{4}$$

where N is the number density of ions, k_β is the Boltzmann constant, T is the temperature and γ_t is the ratio of specific heats for the table material. For the same temperature and number density of ions define a material pressure, energy density, and specific internal energy for material s

$$P_s = N(Z_s + 1)k_\beta T \tag{5}$$

$$E_s = N((Z_s + 1)/(\gamma_s - 1))k_\beta T \tag{6}$$

$$\epsilon_s = E_s/\rho_s = ((Z_s + 1)/(\gamma_s - 1))k_\beta T/M_s \tag{7}$$

The ratios of density, energy density, specific internal energy, and pressure between the actual material (s) and table material (t) are:

$$\rho_t/\rho_s = M_t/M_s \tag{8}$$

$$E_t/E_s = (Z_t + 1)/(Z_s + 1)(\gamma_t - 1)/(\gamma_s - 1) \tag{9}$$

$$\epsilon_t/\epsilon_s = M_s/M_t(Z_t + 1)/(Z_s + 1)(\gamma_s - 1)/(\gamma_t - 1) \tag{10}$$

$$P_t/P_s = (Z_t + 1)/(Z_s + 1) \tag{11}$$

If $(\gamma_s - 1) = (\gamma_t - 1)$ then

$$\rho_t/\rho_s = M_t/M_s \tag{12}$$

$$E_t/E_s = (Z_t + 1)/(Z_s + 1) \tag{13}$$

$$\epsilon_t/\epsilon_s = M_s/M_t(Z_t + 1)/(Z_s + 1) \tag{14}$$

$$P_s/P_t = (Z_s + 1)/(Z_t + 1) \tag{15}$$

Equations (12) to (15) are the scaling ratios. To use the table for material (t) to calculate a pressure for material (s) define ρ_t and ϵ_t as:

$$\rho_t \equiv \rho_s M_t/M_s \tag{16}$$

and

$$\epsilon_t \equiv \epsilon_s(Z_t + 1)/(Z_s + 1)M_s/M_t \tag{17}$$

Use these values of density and specific internal energy in the table for material (t) to find the pressure of material (s).

$$P_s(\rho_s, \epsilon_s) = P_t(\rho_t, \epsilon_t)(Z_s + 1)/(Z_t + 1) \tag{18}$$

To verify the result, write the pressure for material (s) in the form

$$P_s = (\gamma_t - 1)\epsilon_t\rho_t(Z_s + 1)/(Z_t + 1) \tag{19}$$

Substitute equations (16) and (17) into equation (19). Since $(\gamma_t - 1) = (\gamma_s - 1)$, the result is

$$P_s = (\gamma_s - 1)\rho_s \epsilon_s, \tag{20}$$

which is the desired result.

Finally, to calculate $(Z_s + 1)$ and M_s from isotope mass fractions define ν_i^s as the mass fraction of isotope (i) of material (s). Let N_i^s be the local particle number density of isotope (i) of material (s). Also, m_i^s and z_i^s are the atomic weight and number density of isotope (i) of material (s). The average atomic weight and average atomic number of material (s) are given as

$$M_s = \sum_{i=1}^{n} m_i^s N_i^s / N_s \tag{21}$$

and

$$Z_s = \sum_{i=1}^{n} z_i^s N_i^s / N_s \tag{22}$$

where

$$N_s = \sum_{i=1}^{n} N_i^s \tag{23}$$

The local mass fraction of isotope (i) of material (s) is defined as

$$\nu_i^s \equiv m_i^s N_i^s / m_s N_s \tag{24}$$

where

$$\sum_{i=1}^{n} \nu_i^s = 1.0 \tag{25}$$

and n is the total number of isotopes in material (s). From equation (24) the average atomic mass of material (s) is given as follows.

$$\nu_i^s / m_i^s = N_i^s / M_s N_s \tag{26}$$

$$\sum_{i=1}^{n} \nu_i^s / m_i^s = N_s / M_s N_s \tag{27}$$

Therefore

$$M_s = 1 / \sum_{i=1}^{n} \nu_i^s / m_i^s \tag{28}$$

Further

$$N_i^s = M_s N_s \nu_i^s / m_i^s \tag{29}$$

$$(Z_s + 1) = \sum_{i=1}^{n} (z_i^s + 1) N_i^s / \sum_{i=1}^{n} N_i^s$$

$$(Z_s + 1) = \sum_{i=1}^{n} (z_i^s + 1)(\nu_i^s / m_i^s) / \sum_{i=1}^{n} (\nu_i^s / m_i^s)$$

$$(Z_s + 1) = M_s \sum_{i=1}^{n} (z_i^s + 1) \nu_i^s / m_i^s$$

and

$$(Z_s + 1)/M_s = \sum_{i=1}^{n} (z_i^s + 1) \nu_i^s / m_i^s \tag{30}$$

which represents the necessary functions needed to scale all the EOS calculations.

At low temperature a scaling ratio $S_r = M_t/M_s$ has traditionally been used to scale the density and internal energy when using a tabular EOS.

$$\rho_t = \rho_s S_r$$

$$\epsilon_t = \epsilon_s / S_r$$

With the above scaling of the density and and specific internal energy the pressure of the material s is

$$P_s = P_t(\rho_t, \epsilon_t) \tag{31}$$

Equations (12) through (15) are the scaling ratios . If the atomic ionization states Z_s and Z_t are calculated as a function of temperature and density per cycle per zone for each material, then these scaling ratios can be used throughout a calculation to transition from low to high temperatures. At low temperature or temperatures below the Debye temperature $Z_s = Z_t = 0.0$ and the scaling ratios become

$$\rho_t / \rho_s = M_t / M_s$$

$$E_t / E_s = 1.0$$

$$\epsilon_t / \epsilon_s = M_s / M_t$$

$$P_s / P_t = 1.0$$

which are the scaling ratios traditionally used at low temperatures.