

The effective heat of combustion in CFAST isn't a hard number like 1.6E7 J/kg, but rather a function of other species yield inputs. I can justify (rationalize) it as follows: Since in mother nature's world, the heat of combustion is defined as the heat of formation of the products minus the heat of formation of the reactants for any chemical reaction, the inputs are not, in reality, independent inputs.

Thus, there can be inputs for heat of combustion which may be inconsistent with the empirical inputs for species yields. Perhaps we could put a check in the input parser to flag this. Here's how the math works out. From (a corrected) equation (34) of the CFAST Technical Note 1299,

$$\dot{m}_{CO_2} = \dot{m}_f \times \frac{\left(1 + \frac{h_c}{1.32 \times 10^7} - \frac{O/C}{f/C}\right) - \frac{HCl/C + HCN/C + 9 H/C}{f/C}}{1 + S/CO_2 + CO/CO_2} \quad (34)$$

Note from the numerator of this equation that it is possible to for the CO₂ production rate to become negative. Since other rates are a function of the CO₂, the rest of the world goes south too. The above equation implies that to be self-consistent, the following inequality must hold:

$$\left(1 + \frac{h_c}{1.32 \times 10^7} - \frac{O/C}{f/C}\right) \geq \frac{HCl/C + HCN/C + 9 H/C}{f/C}$$

or

$$h_c \geq 1.32 \times 10^7 \left(\frac{8 H/C - 1}{f/C} \right) \quad \text{and} \quad f/C = 1 + H/C + HCl/C + HCN/C + O/C$$

the terms h_c , H/C , and O/C are direct CFAST inputs. The terms HCl/C and HCN/C are defined in the CFAST Technical Note 1299 in equations (36) and (37) in terms of direct CFAST inputs. This must hold for all time points in an input file.

$$\left(1 + \frac{h_c}{1.32 \times 10^7} - \frac{O/C}{f/C}\right) \geq \frac{HCl/C + HCN/C + 9 H/C}{f/C}$$

where $f/C = 1 + H/C + HCl/C + HCN/C + O/C$. Rearranging gives

$$h_c \geq 1.32 \times 10^7 \left(\frac{9 H/C + HCl/C + HCN/C + O/C}{f/C} - 1 \right) \\ \geq 1.32 \times 10^7 \left(\frac{8 H/C + H/C + HCl/C + HCN/C + O/C}{f/C} - 1 \right)$$

Noting that the last four terms in the numerator are equal to $f/C - 1$, this becomes

$$\begin{aligned}
h_c &\geq 1.32 \times 10^7 \left(\frac{8 H/C + f/C - 1}{f/C} - 1 \right) \\
&\geq 1.32 \times 10^7 \left(\frac{8 H/C + f/C - 1}{f/C} - \frac{f/C}{f/C} \right) \\
&\geq 1.32 \times 10^7 \left(\frac{8 H/C - 1}{f/C} \right)
\end{aligned}$$

The definition of f/C in terms of direct CFAST inputs can be expressed noting that

$$\begin{aligned}
HCl/C &= HCl/f \left(\frac{1 + H/C + O/C}{1 - HCl/F - HCN/f} \right) \\
HCN/C &= HCN/F \left(\frac{1 + H/C + O/C}{1 - HCl/F - HCN/f} \right) \\
&= HCl/F \frac{HCN/f}{HCl/f}
\end{aligned}$$

Substituting into the definition of f/C above yields

$$\begin{aligned}
f/C &= 1 + H/C + HCl/C \left(1 + \frac{HCN/f}{HCl/f} \right) + O/C \\
&= 1 + H/C + O/C + HCl/f \left(\frac{1 + H/C + O/C}{1 - HCl/f - HCN/f} \right) \left(1 + \frac{HCN/f}{HCl/f} \right) \\
&= 1 + H/C + O/C + \frac{(1 + H/C + O/C) (HCN/f + HCl/f)}{1 - HCl/f - HCN/f} \\
&= \frac{(1 + H/C + O/C) (1 - HCl/f - HCN/f) + (1 + H/C + O/C) (HCN/f + HCl/f)}{1 - HCl/f - HCN/f} \\
&= \frac{(1 + H/C + O/C) (1 - HCl/f - HCN/f + HCN/f + HCl/f)}{1 - HCl/f - HCN/f} \\
&= \frac{1 + H/C + O/C}{1 - HCl/f - HCN/f}
\end{aligned}$$