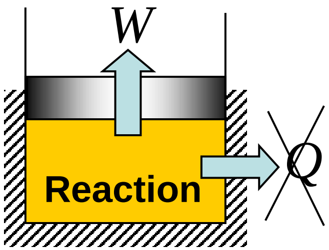
Adiabatic Flame Temperature

Consider the case where the cylinder is perfectly insulated so the process is adiabatic (Q = 0)



$P_2 = P_a$
$T_2 = T_a$

For a constant pressure process, the final products temperature, T_a, is known as the **adiabatic flame temperature** (AFT).

$$Q = \sum_P n_i \bar{h}_i (T_p) - \sum_R n_i \bar{h}_i (T_R) = 0$$

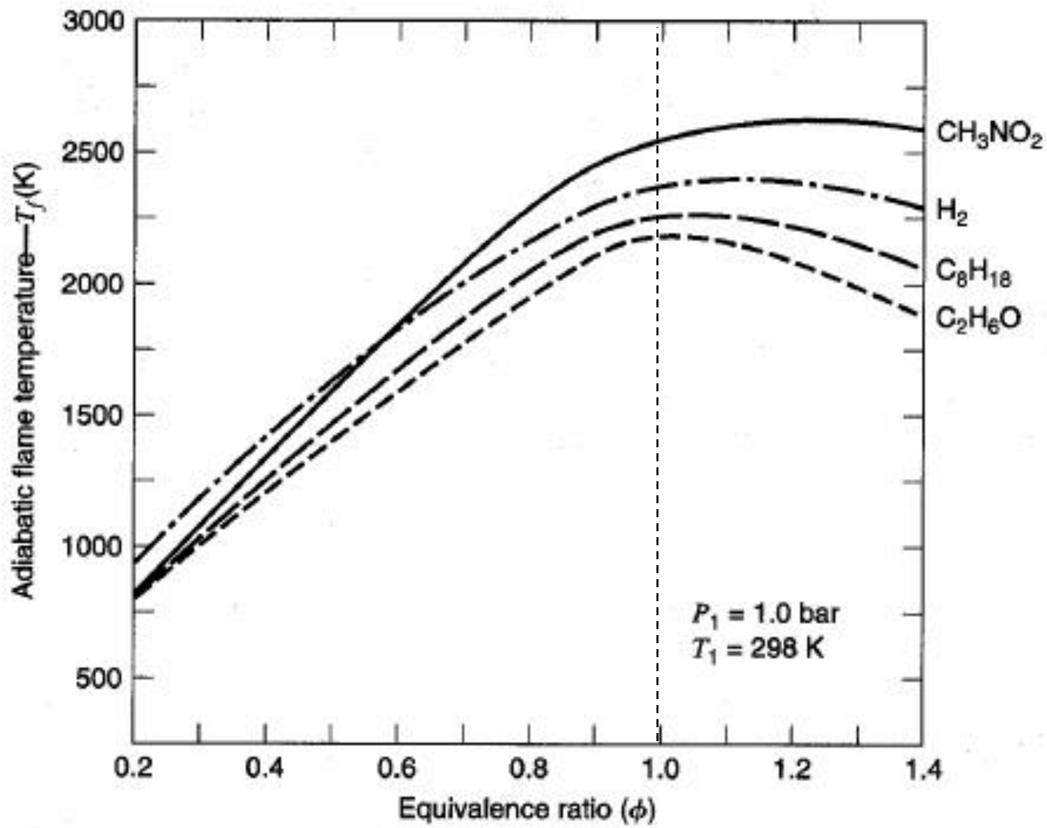
$$\sum_P n_i \bar{h}_i (T_a) = \sum_R n_i \bar{h}_i (T_1)$$

For a given reaction where the n_i's are known for both the reactants and the products, T_a can be calculated explicitly.

Constant Pressure Adiabatic Flame Temperature w/products at equilibrium

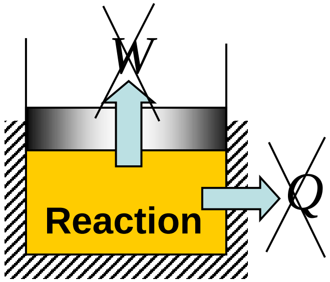
FUEL		$T_{a,\phi=1.0}$ (K)
C_2N_2 (g)	Cyanogen	2596
H_2 (g)	Hydrogen	2383
NH_3 (g)	Ammonia	2076
CH_4 (g)	Methane	2227
C_3H_8 (g)	Propane	2268
C_8H_{18} (l)	Octane	2266
$C_{15}H_{32}$ (l)	Pentadecane	2269
$C_{20}H_{40}$ (g)	Eicosane	2291
C_2H_2 (g)	Acetylene	2540
$C_{10}H_8$ (s)	Naphthalene	2328
CH_4O (l)	Methanol	2151
C_2H_6O (l)	Ethanol	2197
CH_3NO_2 (l)	Nitromethane	2545

Constant Pressure Adiabatic Flame Temperature w/products at equilibrium



Constant Volume Adiabatic Flame Temperature

Consider the case where the piston is fixed and the cylinder is perfectly insulated so the process is adiabatic (Q = 0)



$P_2 = P_{CV}$
$T_2 = T_a$

$$Q = \sum_P n_i \bar{u}_i (T_p) - \sum_R n_i \bar{u}_i (T_R) = 0$$

$$\sum_P n_i \bar{u}_i (T_a) = \sum_R n_i \bar{u}_i (T_1)$$

Note $h = u + pv = u + RT$, so

$$\sum_P n_i (\bar{h}_i (T_a) - \bar{R} T) = \sum_R n_i (\bar{h}_i (T_1) - \bar{R} T)$$

Constant Volume Combustion Pressure

Assuming ideal gas behavior:

$$V_R = V_P$$

$$\frac{n_R \bar{R} T_R}{P_R} = \frac{n_p \bar{R} T_p}{P_p}$$

$$\frac{P_p}{P_R} = \left(\frac{n_p}{n_R}\right)\left(\frac{T_p}{T_R}\right) \quad \rightarrow \quad \frac{P_{CV}}{P_i} = \left(\frac{n_p}{n_R}\right)\left(\frac{T_a}{T_i}\right)$$

For large HCs the mole ratio term is small, e.g., for stoichiometric octane air

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47N_2$$

$$\frac{P_{CV}}{P_i} = \left(\frac{n_p}{n_R}\right)\left(\frac{T_a}{T_i}\right) = \left(\frac{64}{60.5}\right)\left(\frac{T_a}{T_i}\right) = 1.06\left(\frac{T_a}{T_i}\right)$$

For stoichiometric octane-air T_a is 2266K so P_{CV}/P_i = 8.1

Adiabatic Flame Temperature w/Products at Equilibrium

$$C_\alpha H_\beta + (\alpha + \frac{\beta}{4})(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2 + dO_2 + eCO + fH_2$$
$$+ gH + hO + iOH + jNO + kN + \cdots$$

- One can calculate the AFT for the above stoichiometric reaction where the products are at equilibrium.

- Note dissociation in the products will result in a lower AFT since dissociation reactions are endothermic.

- Computer programs are used for these calculations