

# Analysis of hydrogen combustion in a confined volume

Dean Wheeler  
March 2007

variable  $x$  is the volume fraction of fuel gas ( $2/3$  H<sub>2</sub> +  $1/3$  O<sub>2</sub>) in the overall pre-combustion gas mixture:

$$x = \frac{\text{vol}_{\text{fuel\_gas}}}{\text{vol}_{\text{fuel\_gas}} + \text{vol}_{\text{air}}}$$

governing equations:

1. energy conservation
2. mass conservation
3. ideal gas law

$$R_{\text{gas}} := 8.31451 \cdot \frac{\text{J}}{\text{mol} \cdot \text{K}} \quad \text{kJ} := 1000 \cdot \text{J}$$

physical properties:

$$a1 := 3.48283 \quad a2 := 3402 \cdot \text{K} \quad a3 := 3012 \cdot \text{K} \quad a4 := 1353 \cdot \text{K} \quad a5 := 1484 \cdot \text{K}$$

$$u_{\text{air}}(T) := R_{\text{gas}} \cdot \left[ (a1 - 1) \cdot T + a2 \cdot \coth\left(\frac{a3}{T}\right) + a4 \cdot \tanh\left(\frac{a5}{T}\right) \right]$$

$$w1 := 4.0123 \quad w2 := 8414 \cdot \text{K} \quad w3 := 2611 \cdot \text{K} \quad w4 := 1250 \cdot \text{K} \quad w5 := 1169 \cdot \text{K}$$

$$u_{\text{wat}}(T) := R_{\text{gas}} \cdot \left[ (w1 - 1) \cdot T + w2 \cdot \coth\left(\frac{w3}{T}\right) + w4 \cdot \tanh\left(\frac{w5}{T}\right) \right]$$

$$H_{\text{comb}} := 241.82 \cdot \frac{\text{kJ}}{\text{mol}}$$

ambient conditions:  $T_0 := 298 \cdot \text{K} \quad P_0 := 1 \cdot \text{atm}$

energy balance:

$$\Delta e(x, T) := 3 \cdot (1 - x) \cdot (u_{\text{air}}(T) - u_{\text{air}}(T_0)) + 2 \cdot x \cdot (u_{\text{wat}}(T) - u_{\text{wat}}(T_0)) - 2 \cdot x \cdot H_{\text{comb}}$$

guess  $T := 1000 \cdot \text{K}$

results  $T(x) := \text{root}(\Delta e(x, T), T)$

$$P(x) := P_0 \cdot \left(1 - \frac{1}{3} \cdot x\right) \cdot \frac{T(x)}{T_0}$$

Note: these post-combustion temperatures and pressures are probably overestimated because of my neglect of dissociation of product molecules. Also, as heat is lost to surroundings the pressure will drop rapidly. Because there are fewer molecules of gas after the reaction compared to before, if you wait long enough for the product gases to cool back to room temperature, the result will be a partial vacuum.

$x := 0, 0.01.. 1$

