

Heat of combustion, Δh_c

is numerically same as enthalpy of reaction (Δh_R) with the opposite sign

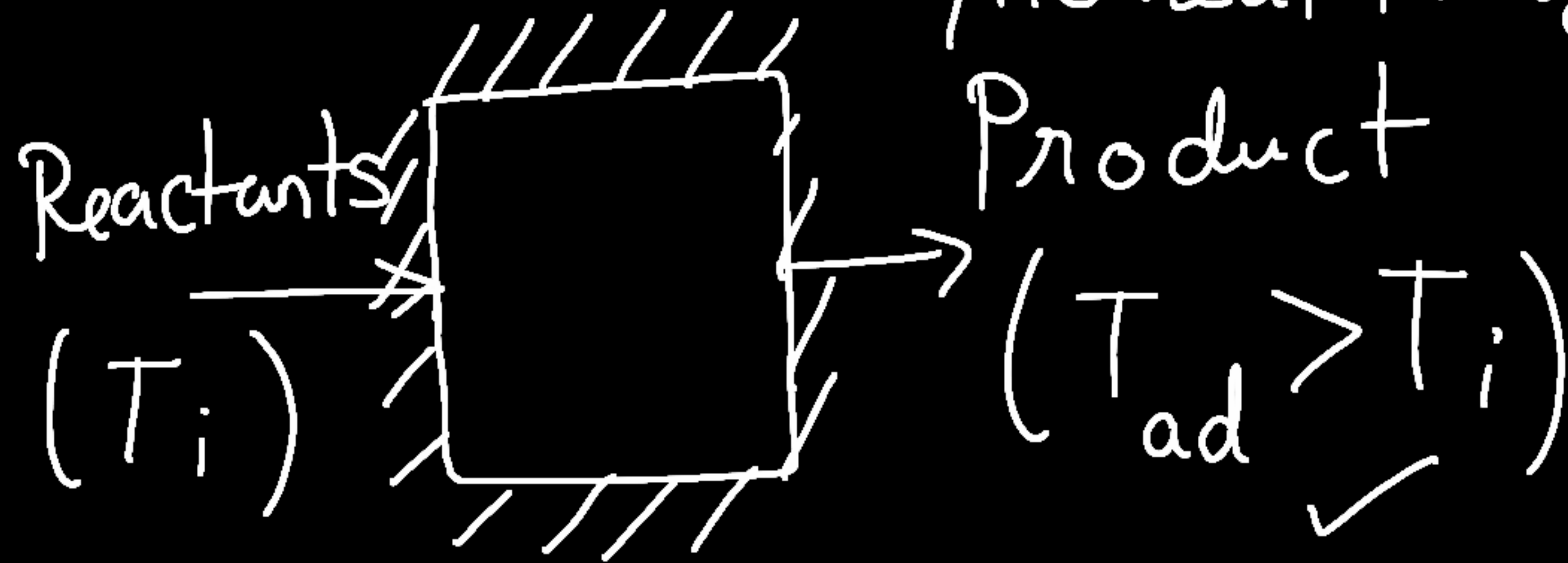
$$\Delta h_c = -\Delta h_R$$

Upper/higher heating value (HHV)
is the Δh_c , assuming all the water in the product is condensed to liquid phase.

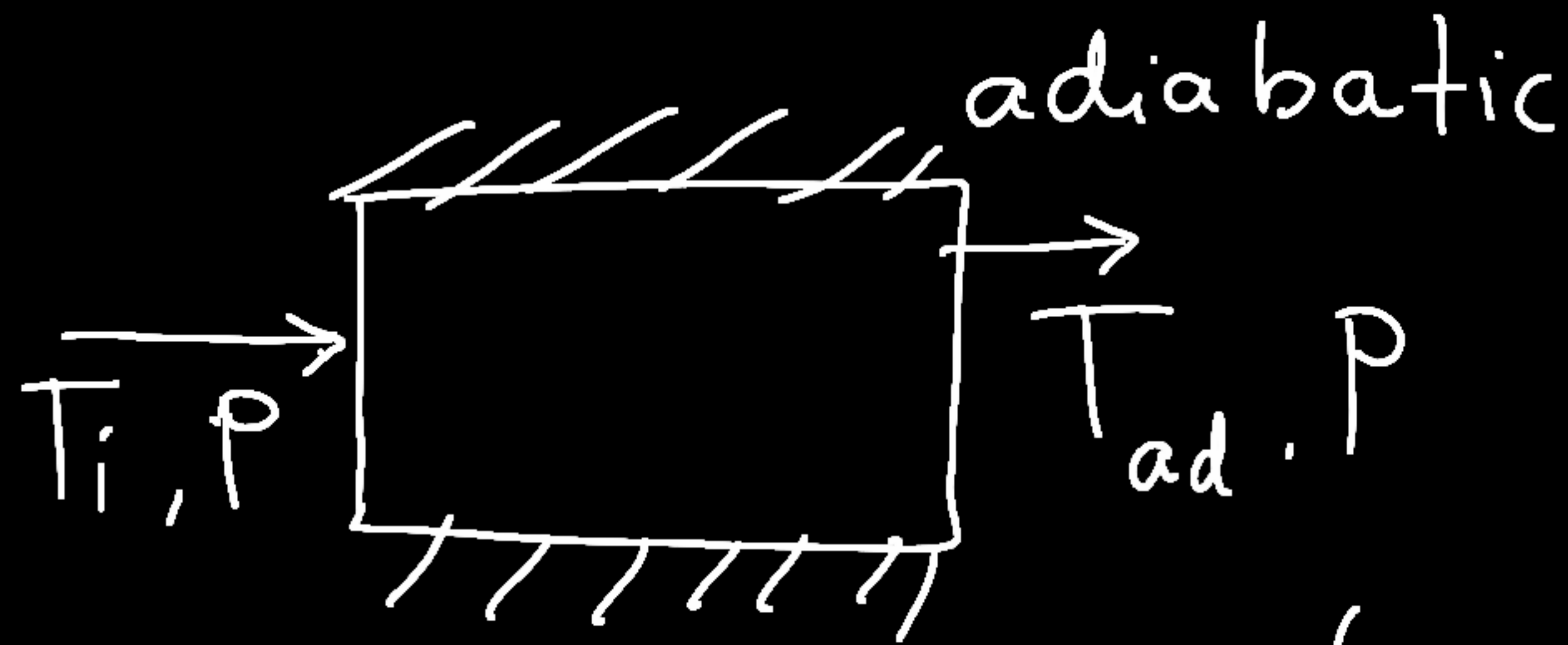
Lower heating value (LHV)
is Δh_c when none of the water is
assumed to be condensed.

$$\text{HHV} > \text{LHV}_{\text{depends}} \\ (5-12\% \text{ fuel.})$$

A diabatic flame temperature (T_{ad})



Constant volume or pressure process.
Rockets/gas turbine engines.



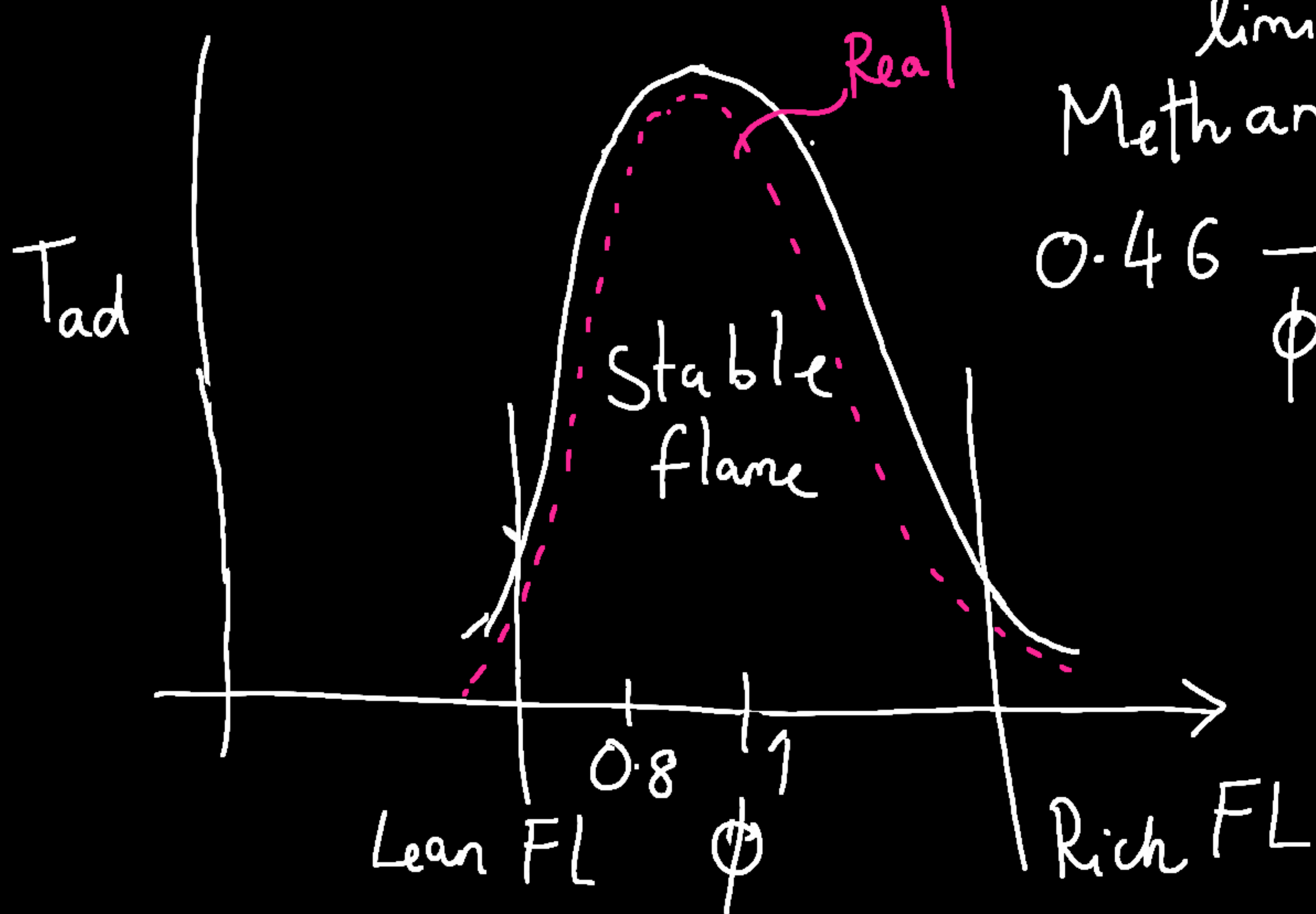
$$H_{\text{reac}}(T_i) = H_{\text{prod}}(T_{ad})$$

"Chemical equilibrium"

T_{ad} V_s ϕ

FL - flammability
limits
Methane

0.46 — 1.64
 ϕ





Example problem: heating values

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

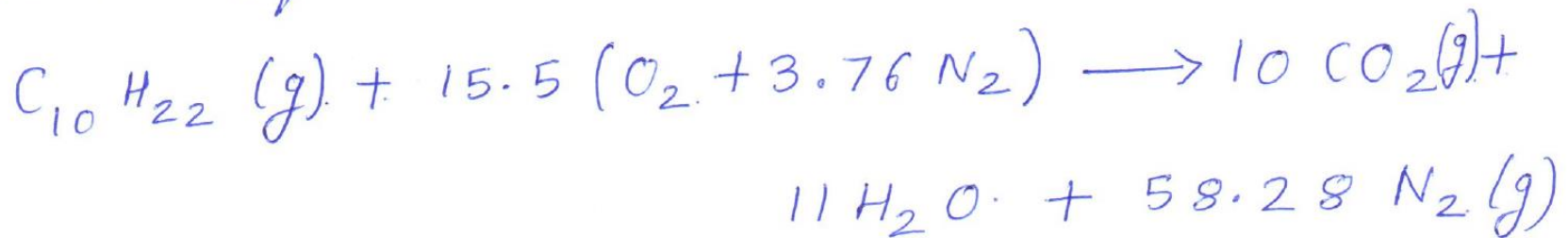
Determine the upper and lower heating values at 298 K of gaseous n-decane, $C_{10}H_{22}$, per Kmole and Kg of fuel. The molecular weight of n-decane is 142 g/mol.

Ex. prob. 2.4 from Turns.

For complete combustion of n-decane, $C_{10}H_{22}$

$$x=10, y=22, \Rightarrow a = x + y/4 = 10 + \frac{22}{4} = 15.5.$$

Chemical equation is.



Heat of combustion, $\Delta H_c = -\Delta H_R = -(H_{prod} - H_{reac})$

$$\Delta H_c = H_{reac} - H_{prod}.$$



Example problem

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The following are obtained from the tables,

$$h_f^\circ \text{C}_{10}\text{H}_{22}(\text{g}) = -249659 \text{ kJ/kmol}$$

$$h_f^\circ \text{O}_2(\text{g}) = h_f^\circ \text{N}_2(\text{g}) = 0$$

$$h_f^\circ \text{CO}_2(\text{g}) = -393546 \text{ kJ/kmol}$$

$$h_f^\circ \text{H}_2\text{O}(\text{g}) = -241845 \text{ kJ/kmol}$$

Lower Heating Value (LHV).

$$H_{\text{reac}} = 1 \times h_f^\circ \text{C}_{10}\text{H}_{22}(\text{g}) + 15.5 \times (h_f^\circ \text{O}_2(\text{g}) + 3.76 h_f^\circ \text{N}_2(\text{g}))$$



Example problem

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Lower Heating Value (LHV).

$$H_{\text{reac}} = 1 \times h_{f, \text{C}_{10}\text{H}_{22}}^{\circ}(\text{g}) + 15.5 \times (h_{f, \text{O}_2}^{\circ}(\text{g}) + 3.76 h_{f, \text{N}_2}^{\circ}(\text{g}))$$

$$H_{\text{reac}} = -249659 \text{ kJ/mol}$$

$$H_{\text{prod}} = 10 \times h_{f, \text{CO}_2}^{\circ}(\text{g}) + 11 \times h_{f, \text{H}_2\text{O}}^{\circ}(\text{g}) + 58.28 \times h_{f, \text{N}_2}^{\circ}(\text{g})$$

$$= 10 \times (-393546) + 11 \times (-241845) + 0$$

$$H_{\text{prod}} = -6595755 \text{ kJ.}$$

$$\Delta H_c = -249659 + 6595755 = +6346096 \text{ kJ.}$$



Example problem

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Since unit mole of $C_{10}H_{22}(g)$ is used, (2)

$$\Delta h_c = 6346096 \text{ kJ/kmol } C_{10}H_{22}(g)$$

$$M_{W C_{10}H_{22}(g)} = 10 \times 12 + 22 \times 1 = 142 \text{ kg/kmol.}$$

$$\Rightarrow \Delta h_c = 6346096 / 142 = \boxed{44690.82 \text{ kJ/kg} = \text{LHV.}}_{C_{10}H_{22}(g)}$$



Example problem

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Higher heating value (HHV).

Here all the water have to be condensed.

$$h_{f,H_2O(g)}^\circ = h_{f,H_2O(l)}^\circ + h_{vap,H_2O}^\circ \quad [h_{vap}^\circ \text{ is the heat of vaporisation} = 44010 \text{ kJ/kmol}]$$

$$h_{f,H_2O(l)}^\circ = h_{f,H_2O(g)}^\circ - h_{vap,H_2O}^\circ$$

$$= -241845 - 44010 = -285855 \text{ kJ/kmol.}$$

$$\therefore H_{prod} = 10 \times h_{f,CO_2(g)}^\circ + 11 \times h_{f,H_2O(l)}^\circ + 58.28 \times h_{f,N_2(g)}^\circ$$

$$= 10 \times (-393546) + 11 \times (-285855) + 0$$

$$= -7079865 \text{ kJ.}$$



Example problem

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$$\Delta H_c = -249659 + 7079865 = 6830206 \text{ kJ}$$

$$\Delta h_c = 6830206 \text{ kJ/kmol}_{\text{C}_{10}\text{H}_{22}(\text{g})}$$

$$\Delta h_c = \frac{6830206}{142} = \boxed{48100.04 \text{ kJ/kg}_{\text{C}_{10}\text{H}_{22}(\text{g})}} = \text{HHV}$$

As from the lectures, $\text{HHV}_{\text{C}_{10}\text{H}_{22}(\text{g})} > \text{LHV}_{\text{C}_{10}\text{H}_{22}(\text{g})}$

In this case, $\text{HHV} = 1.076 \text{ LHV}$.

or HHV is 7.6% higher than LHV.



Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Estimate the constant pressure adiabatic flame temperature for the combustion of Methane-air mixture for equivalence ratios, $\Phi = 1, 0.8$. The pressure is 1 atm and the initial reactant temperature is 298 K. c_p of the product mixture is evaluated at 1200 K.

Prob 2.5. (Example) from Turns. Combustion book. ①
Combustion of Methane



From The tables, the following data are obtained.

Species	$h_{f,i}^\circ$ (kJ/kmol)	$\bar{c}_{p,i}$ (kJ/kmol·K) (@ 1200 K)
CH ₄	-74,831	78.84
CO ₂	-393546	56.21
H ₂ O	-241845	43.87
N ₂	0	33.71
O ₂	0	35.59



Example: adiabatic flame temperature

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Standardized enthalpy of reactant.

$$H_{\text{reac}}(T_{\text{ref}}) = h_{f, \text{CH}_4}^{\circ} + 2h_{f, \text{O}_2}^{\circ} + h_{f, \text{N}_2}^{\circ} \times 7.52$$

$$= -74831 + 0 + 0.$$

$$\Rightarrow H_{\text{reac}}(T_{\text{ref}}) = -74831 \text{ kJ}.$$

For products.

$$H_{\text{prod}}(T = T_{\text{ad}}) = h_{f, \text{CO}_2}^{\circ} + \Delta h_{s, \text{CO}_2}(T_{\text{ad}}) +$$

$$2 \cdot (h_{f, \text{H}_2\text{O}}^{\circ} + \Delta h_{s, \text{H}_2\text{O}}(T_{\text{ad}})) +$$

$$\Delta h_{s, i} = \bar{c}_{p, i}(T_{\text{ad}} - T_{\text{ref}}) \quad 7.52 \cdot (h_{f, \text{N}_2}^{\circ} + \Delta h_{s, \text{N}_2}(T_{\text{ad}}))$$

$$= -393546 + 56.21 \times (T_{\text{ad}} - 298) +$$

$$2 \cdot [-241845 + 43.87 \times (T_{\text{ad}} - 298)]$$

$$+ 7.52 [0 + 33.71 \times (T_{\text{ad}} - 298)]$$



Example: adiabatic flame temperature

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$$\Rightarrow H_{\text{prod}}(T_{\text{ad}}) = -995675.8616 + 397.4492 T_{\text{ad}} \quad (2)$$

For Adiabatic flame temperature,

$$H_{\text{reac}} = H_{\text{prod}}$$

$$\therefore -74831 = -995675.8616 + 397.4492 T_{\text{ad}}$$

$$\Rightarrow \boxed{T_{\text{ad}} = 2316.89 \text{ K}}$$

Adiabatic flame temperature.



Example: adiabatic flame temperature

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For fuel lean case, say $\Psi = 0.8$

$$\frac{(A/F)_s}{(A/F)} = 0.8 \Rightarrow A/F = \frac{(A/F)_s}{0.8} = \frac{17.16}{0.8} = 21.45$$

$$(A/F) = \frac{n_{air}}{n_{fuel}} = \frac{n_{air} M_{W_{air}}}{n_{fuel} M_{W_{fuel}}} = \frac{n_{air}}{n_{fuel}} \frac{28.84}{16} = 21.45$$

$$\frac{n_{air}}{n_{fuel}} = 11.9$$

For 1 mole of fuel (CH_4) $n_{fuel} = 1$

$$n_{air} = 11.9$$

1 ($O_2 + 3.76 N_2$) contains 4.76 moles of air.

\Rightarrow b. ($O_2 + 3.76 N_2$) contains 11.9 moles of air

$$\Rightarrow b = \frac{11.9}{4.76} \times 1 = 2.5$$



Example: adiabatic flame temperature

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\Rightarrow so the chemical equation becomes,

$$\text{CH}_4 + 2.5 (\text{O}_2 + 3.76 \text{N}_2) \longrightarrow \text{CO}_2 + 2 \text{H}_2\text{O} + \frac{1}{2} \text{O}_2 + 9.4 \text{N}_2.$$

$$\begin{aligned} H_{\text{reac}}(T_{\text{ref}}) &= h_{f\text{CH}_4}^\circ + 2.5 (h_{f\text{O}_2}^\circ + 3.76 \cdot h_{f\text{N}_2}^\circ) \quad (3) \\ &= -74831 + 2.5 (0 + 0) = -74831 \text{ KJ.} \end{aligned}$$



Example: adiabatic flame temperature

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$$\begin{aligned}
 H_{\text{prod.}}(T_{\text{ad}}) &= h_{f\text{CO}_2}^{\circ} + \bar{c}_{p\text{CO}_2} (T_{\text{ad}} - 298) + \\
 &+ 2 \cdot [h_{f\text{H}_2\text{O}}^{\circ} + \bar{c}_{p\text{H}_2\text{O}} (T_{\text{ad}} - 298)] + \\
 &+ \frac{1}{2} [h_{f\text{O}_2}^{\circ} + \bar{c}_{p\text{O}_2} (T_{\text{ad}} - 298)] + \\
 &+ 9.4 [h_{f\text{N}_2}^{\circ} + \bar{c}_{p\text{N}_2} (T_{\text{ad}} - 298)] \\
 &= -393546 + 56.21 (T_{\text{ad}} - 298) + \\
 &+ 2 [-241845 + 43.87 (T_{\text{ad}} - 298)] \\
 &+ \frac{1}{2} [0 + 35.59 (T_{\text{ad}} - 298)] \\
 &+ 9.4 [0 + 33.71 (T_{\text{ad}} - 298)]
 \end{aligned}$$



Example: adiabatic flame temperature

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Equating, $H_{\text{reac}}(T_{\text{ref}}) = H_{\text{prod}}(T_{\text{ad}}),$

$$T_{\text{ad}} - 298 = 1676.5$$

$$(\text{or}) T_{\text{ad}} = 1974 \text{ K.}$$

Adiabatic flame temperature decreases for $\Phi = 0.8$.



Example: adiabatic flame temperature

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