Lecture 12 Calculation of flame temperature and combustion product composition

Goal of the lecture: To study the principles and methods for calculating the adiabatic flame temperature and determining the equilibrium composition of combustion products.

Brief lecture notes: This lecture focuses on the thermodynamic analysis of combustion processes, emphasizing the determination of flame temperature and the chemical composition of combustion products. Students will learn how to apply energy balance and equilibrium concepts to combustion reactions, understand the difference between stoichiometric, lean, and rich mixtures, and analyze the effects of dissociation at high temperatures. The lecture also introduces computational approaches to calculate the adiabatic flame temperature, both with and without dissociation, and discusses practical relevance for combustion chambers, engines, and gas turbines.

Main part

Flame temperature is the maximum temperature achieved when fuel and oxidizer react chemically, converting chemical energy into thermal energy. It depends on several factors:

- The type of fuel and oxidizer,
- The air-to-fuel ratio (stoichiometric, lean, or rich),
- Initial temperature and pressure,
- The extent of product dissociation.

The highest possible flame temperature corresponds to adiabatic combustion, where no heat is lost to surroundings.

There are two main types:

1. Adiabatic flame temperature without dissociation – assumes complete combustion and stable products.
2. Adiabatic flame temperature with dissociation – considers chemical equilibrium between products at high temperatures.

Theoretical Basis and Energy Balance

The adiabatic flame temperature (T_f) is obtained from the First Law of Thermodynamics for a steady-flow combustion process:

$$\sum n_r h_r(T_0) + Q = \sum n_p h_p(T_f)$$

For an adiabatic process, $Q = 0$, and the equation simplifies to:

$$\sum n_r h_r(T_0) = \sum n_p h_p(T_f)$$

where

- n_r, n_p– moles of reactants and products,
- h_r, h_p– molar enthalpies at given temperatures $T_0$and T_f.

The reaction enthalpy at standard conditions (ΔH_{298}) is known from tabulated data. To find T_f, one iteratively adjusts temperature until the total enthalpy of products equals that of reactants.

Example: Combustion of Methane

For a stoichiometric mixture:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

At $T_0 = 298\,K$, the reaction enthalpy is approximately $\Delta H_{298} = -890$ kJ/mol.

Assuming all products are at temperature T_f:

$$\sum n_p \int_{298}^{T_f} C_p dT = -\Delta H_{298}$$

From the specific heat capacities of $CO_2$and H_2O, the adiabatic flame temperature for methane with air is typically ≈ 2200–2300 K without dissociation. When dissociation (mainly of CO_2 and H_2O) is considered, $T_f$decreases to ≈ 2000–2100 K.

Equilibrium Composition of Combustion Products

At high temperatures, equilibrium must be established among species such as $CO_2, CO, H_2, H_2O, O_2, N_2$.

For example, in methane combustion, partial dissociation occurs through reactions like:

$$CO_2 \rightleftharpoons CO + \frac{1}{2}O_2, H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2$$

The equilibrium constant (Kp) for each reaction depends on temperature:

$$K_p = \frac{(p_{CO})(p_{O_2})^{1/2}}{p_{CO_2}}$$

These constants can be obtained from thermodynamic tables or calculated from Gibbs free energy data. Solving the equilibrium equations allows determination of the mole fractions of each component in the combustion products.

Factors Affecting Flame Temperature

Factor	Effect on Flame Temperature	Explanation
Fuel type	Higher for hydrogen, lower for hydrocarbons	H_2 releases more energy per mass
Air-to-fuel ratio	Maximum at stoichiometric ratio	Excess air or fuel lowers T_f
Initial temperature	Increases $T_f$linearly	Preheating of air/fuel increases efficiency
Pressure	Slightly increases T_f	Higher pressure suppresses dissociation
Dissociation	Decreases T_f	Endothermic dissociation absorbs part of heat

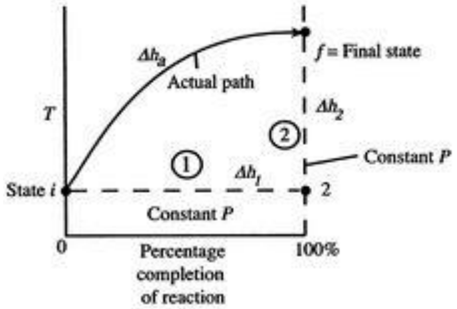

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Figure 1: Dependence of adiabatic flame temperature on the equivalence ratio (ϕ).

1.Energy balance for adiabatic combustion:

$$\sum n_r h_r(T_0) = \sum n_p h_p(T_f)$$

2. Equilibrium constant (Kp):

$$K_p = \frac{\prod (p_i)^{\nu_i}}{\prod (p_j)^{\nu_j}}$$

Questions for Self-Control

1. What is meant by adiabatic flame temperature and how is it determined?
2. How does dissociation of combustion products affect the flame temperature?
3. What factors influence the equilibrium composition of combustion products?
4. How does the air-to-fuel ratio affect the adiabatic flame temperature?
5. Why is accurate flame temperature calculation important for engine and furnace design?

Literature

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