Calculate The Adiabatic Flame Temperature Of Propane (c3h8) Burned In Stoichiometric Air At 25c, 1atm,

Calculate The Adiabatic Flame Temperature Of Propane (c3h8) Burned In Stoichiometric Air At 25°C, 1atm

Understanding the adiabatic flame temperature of propane (C_3H_8) when burned in stoichiometric air at standard conditions is essential for engineers, chemists, and environmental scientists working in combustion analysis, energy production, and emissions control. This article provides a comprehensive overview of how to calculate this temperature, including the fundamental concepts, step-by-step methodology, and practical considerations.

What Is The Adiabatic Flame Temperature?

The adiabatic flame temperature (AFT) is the maximum temperature achievable during combustion when no heat is lost to the surroundings. It is a theoretical value that assumes perfect insulation, meaning all the heat generated from the chemical reaction contributes solely to raising the temperature of the combustion products.

Understanding the AFT of propane in stoichiometric air is crucial because:

- It helps in designing efficient combustion systems.
- It aids in predicting pollutant formation, such as NO_x gases.
- It informs safety protocols by identifying maximum temperature limits.

Fundamental Concepts for Calculating AFT of Propane

Before diving into calculations, it is important to grasp key concepts:

Stoichiometric Combustion

- The ideal combustion process where fuel reacts with exactly enough oxygen to produce complete combustion products (CO_2 and H_2O).
- No excess air or oxygen remains after the reaction.

Combustion Reaction of Propane

- The chemical reaction for propane in excess oxygen is:

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

- When burned in air, which contains approximately 21% oxygen and 79% nitrogen by volume, nitrogen acts as an inert diluent, absorbing some heat and affecting the final temperature.

Standard Conditions

- Initial temperature, T_initial = 25°C (298 K)
- Pressure = 1 atm

Assumptions in Calculation

- The process occurs adiabatically (no heat loss).
- Complete combustion.
- Ideal gas behavior.
- Constant specific heats over temperature range or temperature-dependent specific heats for accuracy.

Step-by-Step Methodology to Calculate AFT of Propane

Calculating the adiabatic flame temperature involves energy balance equations considering the heat released during combustion and the heat capacity of products.

Step 1: Write the Combustion Reaction and Determine Stoichiometric Air Requirement

- The combustion of propane with pure oxygen:

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

- Since air contains 21% O_2, the amount of air needed per mol of propane:

Air requirement = 5 mol O_2 / 0.21 ≈ 23.81 mol air

This defines the stoichiometric air-to-fuel ratio.

Step 2: Calculate the Heat of Reaction (ΔH_combustion) at Standard Conditions

- Use standard enthalpy of formation (ΔH_f°) values:

Substance	ΔH_f° (kJ/mol)
C_3H_8	-103.8
CO_2	-393.5
H_2O (liquid)	-285.8
H_2O (gas)	-241.8

- Since water is produced as vapor at high temperature, use ΔH_f° for gaseous water.

- Enthalpy change per mol of propane:

$$\Delta H_{combustion} = [3 \times \Delta H_f^\circ(CO_2) + 4 \times \Delta H_f^\circ(H_2O)] - \Delta H_f^\circ(C_3H_8)$$

$$\Delta H_{combustion} = [3 \times (-393.5) + 4 \times (-241.8)] - (-103.8)$$

$$\Delta H_{combustion} = [-1180.5 - 967.2] + 103.8 = -2044.9 + 103.8 = -1941.1 \text{ kJ/mol}$$

- The negative sign indicates exothermic reaction releasing heat.

Step 3: Adjust for Complete Combustion in Air

- Since air contains nitrogen, which does not participate in the reaction but absorbs heat, include it in the energy balance.

- For each mol of propane, the total moles of gases after combustion are:

- 3 CO_2
- 4 H_2O vapor
- Nitrogen: 23.81 mol air × 0.79 ≈ 18.8 mol N_2

- Total moles of products: 3 + 4 + 18.8 ≈ 25.8 mol

Step 4: Calculate the Heat Capacity of Combustion Products

- The adiabatic flame temperature is found where the heat released equals the heat required to raise the temperature of the products:

$$Q_{released} = \Sigma\ n_i \times C_{p,i} \times (T_{final} - T_{initial})$$

- For simplicity, assume average constant specific heats (C_p) over the temperature range, or use temperature-dependent data for higher accuracy.

- Approximate average specific heats (kJ/mol·K):

Gas	C_p (approximate) at high T
CO_2	0.844
H_2O vapor	1.996
N_2	1.039

- Total heat capacity per mol of products:

$$C_{total} = (3 \times 0.844) + (4 \times 1.996) + (18.8 \times 1.039)$$

$$C_{total} \approx 2.532 + 7.984 + 19.52 \approx 30.036 \text{ kJ/K}$$

Step 5: Calculate the Adiabatic Flame Temperature (T_{ad})

- Set heat released equal to heat absorbed:

$$\Delta H_{combustion} = C_{total} \times (T_{ad} - T_{initial})$$

- Rearranged:

$$T_{ad} = T_{initial} + (|\Delta H_{combustion}|) / C_{total}$$

- Plugging in values:

$$T_{ad} = 298 \text{ K} + 1941.1 \text{ kJ} / 30.036 \text{ kJ/K} \approx 298 + 64.66 \approx 362.66°C$$

- Convert to Celsius:

$$T_{ad} \approx 362.66°C$$

This is a simplified estimate; more accurate calculations involve integrating temperature-dependent specific heats and considering dissociation effects at high temperatures.

Refining the Calculation for Higher Accuracy

To improve precision:

- Use temperature-dependent specific heat data from thermodynamic tables.
- Incorporate dissociation effects at high temperatures, which can lower the

flame temperature.
- Apply numerical methods or specialized software (like Cantera or CHEMKIN).

Practical Considerations and Applications

- Actual flame temperatures are often lower than the theoretical adiabatic flame temperature due to heat losses, incomplete combustion, and other factors.
- Engineers use the AFT to optimize burner design, select materials, and control emissions.
- Understanding the maximum achievable temperature helps in assessing the formation of nitrogen oxides (NO_x), which are sensitive to temperature.

Conclusion

Calculating the adiabatic flame temperature of propane burned in stoichiometric air at 25°C and 1 atm involves understanding the combustion reaction, calculating the heat released, and applying energy balance principles. While simplified calculations provide a good approximation, detailed thermodynamic data and computational tools can enhance accuracy, essential for practical applications in energy systems, environmental management, and safety protocols.

Key Takeaways:

- The adiabatic flame temperature of propane in ideal conditions is approximately 363°C based on simplified calculations.
- Real-world flame temperatures are typically lower due to heat losses and incomplete combustion.
- Accurate determination requires detailed thermodynamic data and consideration of high-temperature phenomena.

Understanding these principles enables professionals to design safer, more efficient combustion systems and predict environmental impacts effectively.

Frequently Asked Questions

What is the adiabatic flame temperature of propane (C_3H_8) burned in stoichiometric air at 25°C and 1 atm?

The adiabatic flame temperature of propane in stoichiometric air at 25°C and 1 atm is approximately 2,050°C to 2,150°C, depending on specific conditions

and calculation methods.

How do you calculate the adiabatic flame temperature of propane in stoichiometric combustion?

The calculation involves balancing the combustion reaction of propane with oxygen and nitrogen, then applying energy conservation principles to determine the temperature at which the heat released equals the heat absorbed by the combustion products, often using specific heat capacities and enthalpy data.

What is the chemical reaction for the complete combustion of propane in air?

The balanced chemical reaction is $C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2$.

Why is the adiabatic flame temperature of propane important in engineering applications?

It helps in designing combustion systems for optimal efficiency and safety by providing the maximum achievable temperature under ideal conditions without heat loss.

What factors influence the adiabatic flame temperature of propane?

Factors include initial temperature, pressure, mixture stoichiometry, heat capacities of combustion products, and heat losses; assumptions of perfect insulation lead to the adiabatic condition.

How does changing the air-to-fuel ratio affect the adiabatic flame temperature of propane?

Burning with excess air (lean mixture) lowers the flame temperature, while stoichiometric or rich mixtures increase it; however, for stoichiometric combustion, the temperature is maximized.

Can the adiabatic flame temperature of propane be calculated analytically?

Yes, using thermodynamic data, heat capacities, and combustion enthalpies, the adiabatic flame temperature can be estimated analytically with appropriate equations and iterative methods.

What assumptions are typically made when calculating the adiabatic flame temperature of propane?

Assumptions include complete combustion, no heat loss, constant specific heats over temperature range, and ideal gas behavior of combustion products.

How does initial temperature (25°C) influence the adiabatic flame temperature calculation for propane?

The initial temperature affects the energy balance; starting at 25°C means the calculation accounts for this initial thermal energy, resulting in a slightly lower flame temperature compared to calculations assuming higher initial temperatures.

What are common methods or tools used to compute the adiabatic flame temperature of propane?

Common methods include thermodynamic calculations using heat capacity data, software tools like REFPROP or combustion calculators, and iterative numerical techniques to solve for temperature where energy balance is satisfied.

Additional Resources

Calculate The Adiabatic Flame Temperature Of Propane (C3H8) Burned In Stoichiometric Air At 25°C, 1 atm

Understanding the adiabatic flame temperature of hydrocarbon fuels like propane (C3H8) is fundamental in combustion science, energy engineering, and environmental management. This parameter signifies the maximum temperature achievable during complete combustion under idealized, adiabatic conditions—meaning no heat is lost to the surroundings. Accurately calculating this temperature provides insights into energy efficiency, pollutant formation, and thermal management in practical applications such as residential heating, industrial processes, and internal combustion engines.

This article offers a comprehensive examination of the process involved in calculating the adiabatic flame temperature of propane burned in stoichiometric air at standard conditions (25°C and 1 atm). It covers the fundamental principles of combustion chemistry, thermodynamic considerations, detailed step-by-step calculation procedures, and analytical insights into the factors influencing the flame temperature.

Understanding the Fundamentals of Combustion and Flame Temperature

The Significance of Flame Temperature in Combustion

The flame temperature of a fuel-air mixture is an essential indicator of the energy release and thermal environment during combustion. It influences:
- Efficiency of heat transfer processes
- Formation of pollutants such as NOx
- Material selection for combustion chambers
- Emission control strategies

Maximum theoretical temperatures are achieved under adiabatic conditions with complete combustion, which neglects heat losses and incomplete reaction pathways.

What Is the Adiabatic Flame Temperature?

The adiabatic flame temperature (T_ad) is the temperature attained by the combustion products when all the chemical energy of the fuel is converted into sensible heat without any heat transfer to surroundings. It depends on:
- The chemical composition of the fuel
- The equivalence ratio (for stoichiometric conditions, ratio equals 1)
- Initial temperature and pressure
- Specific heats of combustion products

In practical scenarios, actual flame temperatures are often lower due to heat losses and incomplete combustion, but the adiabatic temperature provides an upper limit for thermal analysis.

Chemical Composition of Propane and Combustion Reaction

Propane (C3H8): Properties and Combustion Characteristics

Propane is a hydrocarbon with the molecular formula C3H8, frequently used as a fuel for heating, cooking, and transportation. Its combustion in oxygen (or air) releases energy, primarily through the oxidation of carbon and hydrogen.

Stoichiometric Combustion Reaction

Under ideal conditions, complete combustion of propane with oxygen can be represented as:

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

However, since combustion in air involves nitrogen, the actual reaction includes nitrogen as an inert diluent. The complete combustion reaction with air (which contains approximately 21% O_2 and 79% N_2 by volume) can be written as:

$C_3H_8 + 5O_2 + (20.9/100)\times(\text{moles of } O_2)\times N_2 \rightarrow \text{products}$

To account for the nitrogen, the reaction is commonly scaled to include the nitrogen present in stoichiometric air:

$C_3H_8 + 5O_2 + 19.1N_2 \rightarrow 3CO_2 + 4H_2O + 19.1N_2$

This ratio reflects the fact that for every mole of oxygen, approximately 3.76 moles of nitrogen are present in air (since 79% N_2 / 21% $O_2 \approx 3.76$).

Thermodynamic Principles and Calculation Approach

Energy Balance in Adiabatic Combustion

The core principle underpinning the calculation of T_ad is conservation of energy: the heat released by combustion heats the products from the initial temperature (25°C) to the flame temperature, assuming no heat loss.

Mathematically:

Q_released = Q_absorbed

Where:
- Q_released is the heat of combustion (enthalpy of reaction)
- Q_absorbed is the sum of sensible heats of products at T_ad

Enthalpy of Reaction and Specific Heats

The heat of reaction (ΔH°_reaction) at standard conditions is known from thermodynamic tables. The temperature-dependent sensible heats (Cp) of the products are integrated over the temperature range to relate enthalpy changes:

$$\Delta H = \int Cp(T)\, dT$$

In practice, the calculation involves iterative methods or software tools because Cp varies with temperature.

Step-by-Step Calculation of Adiabatic Flame Temperature

1. Gather Thermodynamic Data

- Standard enthalpy of formation (ΔH_f°) for all reactants and products
- Specific heats (Cp) of products as functions of temperature (often polynomial fits or tabulated data)
- Heat of combustion of propane ($\Delta H_{combustion}$)

Sample data:
- ΔH_f° (C_3H_8): -103.8 kJ/mol
- ΔH_f° (CO_2): -393.5 kJ/mol
- ΔH_f° (H_2O, vapor): -241.8 kJ/mol

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2. Write the Energy Balance Equation

The total heat released per mole of propane is:

$$Q = \Delta H^\circ_{reaction}$$

Expressed as:

$$Q = [3 \times \Delta H_f^\circ(CO_2) + 4 \times \Delta H_f^\circ(H_2O)] - [\Delta H_f^\circ(C_3H_8)]$$

Plugging in values:

$$Q = [3 \times (-393.5) + 4 \times (-241.8)] - (-103.8) = (-1180.5 - 967.2) + 103.8 = -2044.9 + 103.8 = -1941.1 \text{ kJ/mol}$$

The negative sign indicates heat release.

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3. Establish the Temperature-Dependent Sensible Heat of Products

Since the combustion products start at 25°C (298 K), and the flame temperature T_{ad} is unknown, the sensible heat ($Q_{sensible}$) is:

$$Q_{sensible} = \sum n_i \times \int_{298K}^{T_{ad}} C_{p,i}(T)\, dT$$

Where:
- n_i are mole amounts of each species
- $C_{p,i}(T)$ are temperature-dependent specific heats

For simplicity, Cp values are often approximated as constant over the temperature range or fitted with polynomial equations.

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4. Set Up the Energy Balance Equation

Assuming ideal gas behavior and constant Cp (or using polynomial fits), the energy balance becomes:

$$Q = \sum n_i \times \int_{298K}^{T_{ad}} C_{p,i}(T)\, dT$$

Given the initial temperature (25°C), the equation reduces to:

$$\Delta H_{combustion} = \sum n_i \times \int_{298K}^{T_{ad}} C_{p,i}(T)\, dT$$

By solving this equation for T_{ad}, the adiabatic flame temperature is found.

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5. Iterative Solution or Computational Approach

Because Cp varies with temperature, iterative methods or software tools like MATLAB, EES (Engineering Equation Solver), or thermodynamics software are typically used. The process involves:
- Assuming an initial T_{ad} estimate
- Calculating the total sensible heat
- Comparing with the heat released
- Adjusting T_{ad} until convergence

Practical Calculation Example and Approximate

Results

Using typical average Cp values for combustion products:
- $Cp(CO_2) \approx 37$ J/mol·K
- $Cp(H_2O$ vapor$) \approx 33$ J/mol·K
- $N_2 \approx 29$ J/mol·K

Calculating the total heat capacity:

$Q_{total} = (3 \text{ mol} \times 37 + 4 \text{ mol} \times 33 + 19.1 \text{ mol} \times 29)$ J/K
$= (111 + 132 + 553.9)$ J/K
$= 796.9$ J/K

The temperature rise from 25°C (298 K) to T_{ad}:

$\Delta T = Q / C_{p,total} \approx (1941.1 \text{ kJ}) / (0.7969 \text{ kJ/K}) \approx 2434$ K

Adding the initial temperature:

$T_{ad} \approx 298$ K + 2434 K ≈ 2732 K

This approximate calculation suggests an adiabatic flame temperature near 2730 K (~2457°C).

Note: More precise calculations incorporating temperature-dependent Cp and detailed thermodynamic data typically yield flame temperatures in the range of 1980°C to 2200°C for propane combustion under ideal conditions.

Influencing Factors and Real-World Considerations

Impact of Initial Conditions

- Initial Temperature: Higher initial temperatures slightly increase T_{ad}.
- Initial Pressure: Elevated pressure can affect gas densities and heat capacities, subtly influencing flame temperature.

Effect of Combustion Stoichiometry

- Burning in stoichiometric air maximizes flame temperature.
- Excess air (lean mixture) reduces flame temperature due to heat absorption by excess oxygen.
- Rich mixtures (excess fuel) produce lower flame temperatures due to

incomplete combustion and heat losses.

Heat Losses and Practical Limitations

Real flames are not adiabatic; heat losses through radiation, convection, and conduction lower actual

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