



Wydział Mechaniczny Energetyki i Lotnictwa

Politechnika Warszawska

course
MKWS



Thermal cycle of a coal-gas fired coke oven
and its enviromental impact

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Contents

| | |
|---------------------------------|---|
| 1. Introduction | 3 |
| 2. Theoretical knowledge | 3 |
| 3. Model | 5 |
| 4. Python code | 6 |
| 5. Results | 6 |
| 6. Conclusions | 8 |
| 7. References | 8 |

1. Introduction

The combustion of coal gas within the thermal cycle of a coke oven represents a critical process in the broader context of industrial energy systems, particularly in the metallurgical sector. Coke ovens are integral to the production of coke, a carbon-rich material derived from coal through pyrolysis. Coke serves as a fundamental reducing agent and energy source in blast furnace operations, which are essential for the production of pig iron — the primary precursor to steel.

As of recent global estimates, annual steel production exceeds 1.8 billion metric tons, reflecting the continuing demand for steel in construction, manufacturing, transportation, and numerous other sectors. In light of increasing environmental concerns and the need for energy optimization, the study of coal gas combustion within the coke oven cycle offers valuable insights into improving thermal efficiency and reducing emissions in steel production.

During the coke-making process the gas obtained from the coal pyrolysis, later referred as coal-gas, is often burned directly after various cleaning process, to keep the oven running. We can evaluate the heat generated in typical coke-oven setting during this process. This can be done simply by using CANTERA python package, which is ultimately the goal of this project. We will also analyze the emission profile from such, reaction, based on the equivalence ratio.

2. Theoretical knowledge

According to *Koksownictwo cz.2* by Aleksander Karcz, typical composition of purified coal gas include

| | | |
|------------------------|---|-----------|
| CH_4 | - | 23 ÷ 28 |
| C_nH_m | - | 2 ÷ 4 |
| H_2 | - | 53 ÷ 59 |
| CO | - | 6 ÷ 10 |
| CO_2 | - | 2 ÷ 4 |
| N_2 | - | 3 ÷ 8 |
| O_2 | - | 0.2 ÷ 0.8 |

Figure 2.1. Composition limits of the mixture [%]

2. Theoretical knowledge

Where C_nH_m mean various higher-order carbohydrates, mainly ethane and ethylene. Thus, our gas mixture will be approximated as

| Component | Volume Fraction [%] |
|-------------------------------|---------------------|
| C ₂ H ₆ | 1.5 |
| C ₂ H ₄ | 1.5 |
| CH ₄ | 25.0 |
| H ₂ | 56.0 |
| CO | 8.0 |
| CO ₂ | 3.0 |
| O ₂ | 0.5 |
| N ₂ | 4.5 |
| Total | 100.0 |

Table 2.1. Normalized composition of the simulated fuel gas mixture.

The coking heat, defined as the amount of heat per kg of coal needed to finish the process of coke-forming (*Koksownictwo cz.1*), is as follows

$$Q_w = Q_s \cdot \frac{100 - W_t^r}{100} + i_w \cdot \frac{W_t^r}{100} \quad \left[\frac{\text{kJ}}{\text{kg}} \right] \quad (1)$$

- Q_w – heat required for coking moist coal feedstock [kJ/kg of moist coal],
- Q_s – heat required for coking dry coal feedstock [kJ/kg of dry coal],
- W_t^r – total moisture content in the coal mixture [%],
- i_w – enthalpy of steam leaving the coking chamber [kJ/kg of steam].

Which by substituting average values $Q_s = 1415 \text{ kJ/kg}$ and $i_w = 3768 \text{ kJ/kg}$ give us

$$Q_w = 4,187 \cdot (338 + 5,6 \cdot w_t^r) \quad [\text{kJ/kg}] \quad (2)$$

Which in turn give us for dry coal

$$Q_w = 1,415 \frac{\text{MJ}}{\text{kg}}$$

According to [1] the gases leave the oven at $\approx 1400\text{K}$ and are combusted at around $T_0 = 1100\text{K}$ and atmospheric pressure, which will be thus our starting conditions.

3. Model

The enthalpy change, denoted as Δh , represents the difference in specific enthalpy (per unit mass) between the reactants and products during a chemical reaction:

$$\Delta h = h_{\text{reactants}} - h_{\text{products}}$$

In the context of combustion at constant pressure, this difference corresponds to the amount of thermal energy released or absorbed by the system. A positive value indicates energy release (exothermic reaction), while a negative value indicates energy absorption (endothermic reaction).

In the simulation, the enthalpy change is computed as:

$$\Delta h = h_i - h_f$$

where:

- h_i is the specific enthalpy before combustion (initial state),
- h_f is the specific enthalpy after combustion (final equilibrium state).

This value is typically reported in MJ/kg

The equivalence ratio, denoted by ϕ , is a measure of the fuel-to-oxidizer ratio in a combustion system compared to the stoichiometric ratio:

$$\phi = \frac{(F/O)_{\text{actual}}}{(F/O)_{\text{stoichiometric}}}$$

where:

- $(F/O)_{\text{actual}}$ is the actual fuel-to-oxidizer ratio in the mixture,
- $(F/O)_{\text{stoichiometric}}$ is the fuel-to-oxidizer ratio required for complete combustion.

Cantera determines the adiabatic flame temperature by conserving enthalpy during the combustion process at constant pressure. The steps are:

1. Set the initial temperature T_0 , pressure P_0 , and mixture composition at a given ϕ .
2. Use the method `equilibrate('HP')` to solve for the final equilibrium state under constant enthalpy (H) and pressure (P).
3. The resulting temperature after equilibrium is the adiabatic flame temperature, T_{ad} .

$$T_{\text{ad}} = T \quad \text{such that} \quad H(T_0, \text{mixture}) = H(T_{\text{ad}}, \text{products})$$

This model simulates the combustion behavior of a previously defined gas using Cantera and the `gri30.yaml` mechanism. The oxidizer is dry air (21% O_2 , 79% N_2).

The simulation computes:

1. Adiabatic flame temperature via `equilibrate('HP')`
2. Enthalpy difference between pre- and post-combustion states (MJ/kg)
3. Pollutant emissions (ppm): CO, CO₂, NO_x (NO, NO₂, N₂O)
4. Lower Heating Value (LHV) in MJ/kg and MJ/nm³

The results are plotted against ϕ to analyze combustion efficiency, thermal output, and emission characteristics as a function of mixture richness or leanness.

4. Python code

The code used for calculating mentioned cases was written in Python using Cantera package. The code can be found in the repository: <https://github.com/Torygg090/MKWS>

5. Results

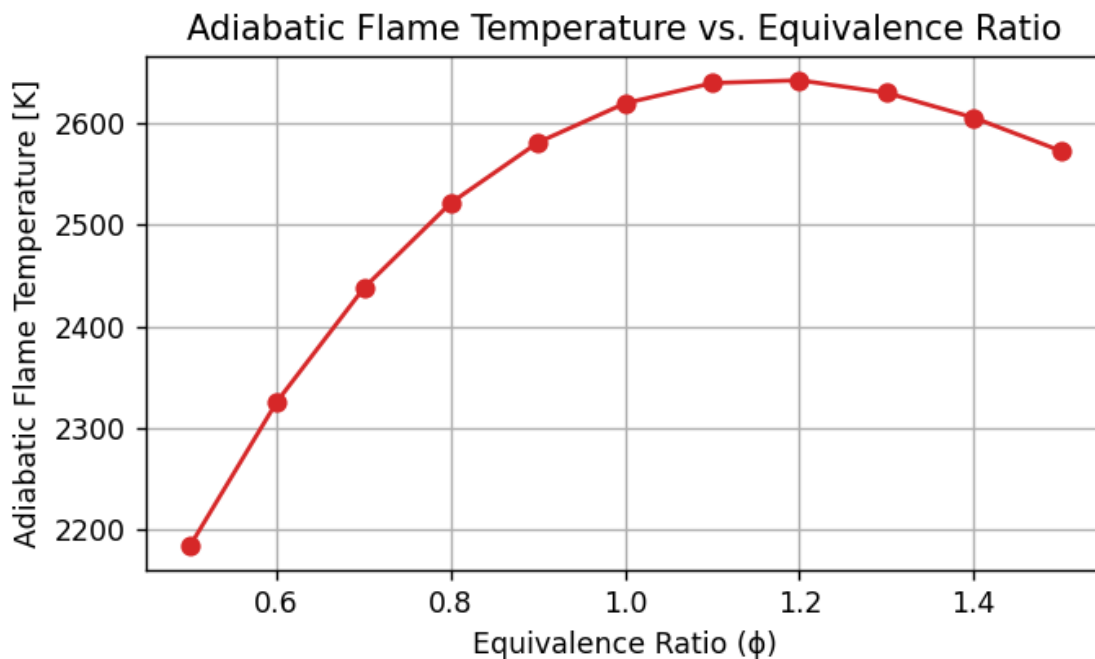
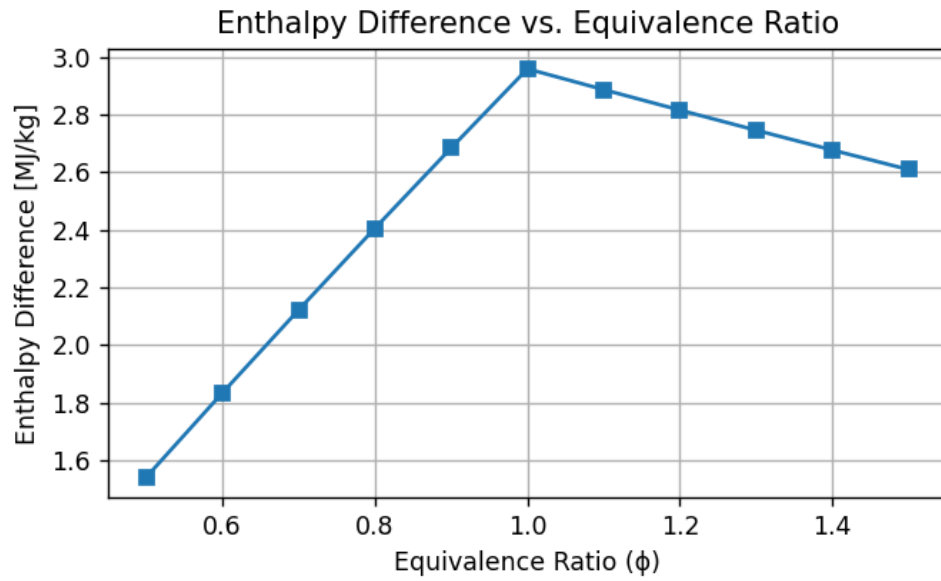
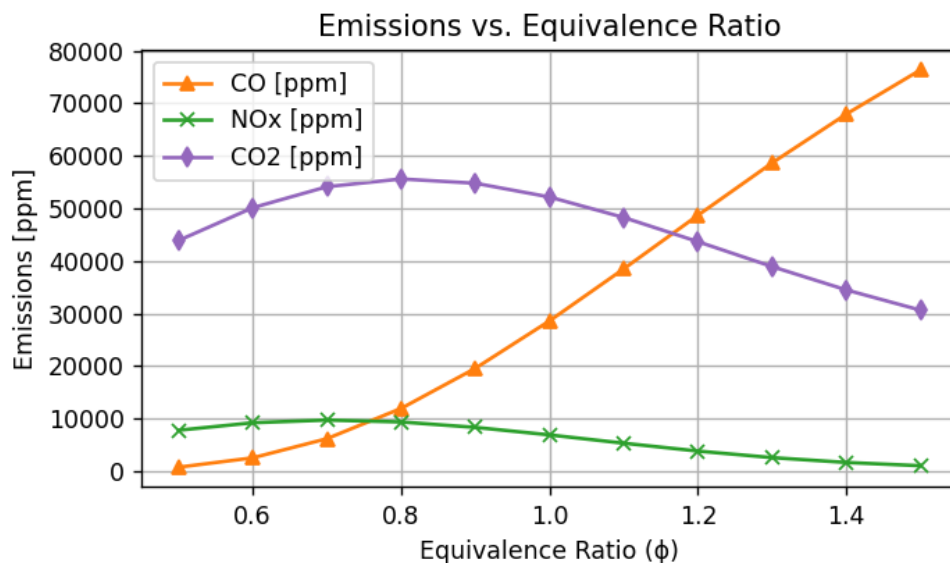


Figure 5.1. Adiabatic Flame Temperature vs. Equivalence Ratio

**Figure 5.2.** Enthalpy Difference vs. Equivalence Ratio**Figure 5.3.** Emissions vs. Equivalence Ratio

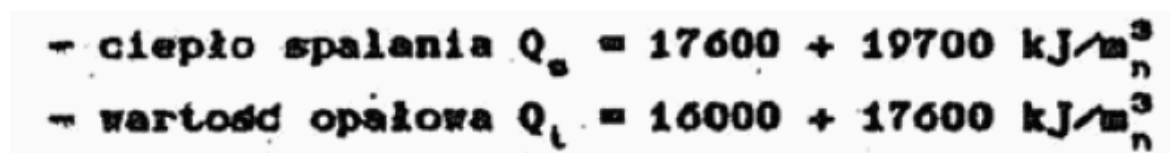
6. Conclusions

According to [1], 1kg of coal, depending on the grade of the fuel, release around 0,23kg of coal gas. If we multiply the maximum enthalpy change by this value we get $\Delta h = 0,69 \frac{MJ}{kg}$, which is over **two times lower than the amount needed to produce the gas**. We must also acknowledge, that what we have here is the most ideal case. We did not model various other heat losses, such as

- Heat losses from the oven to surroundings
- The enthalpy of gasses leaving the combustion chamber
- Potential energy needed to evaporate moisture within coal

The overall conclusion is in line with the literature, as stated again in [1]. We also see, that the maximal adiabatic flame temperature reaches around 2625K, and that in this case, we have to be wary of toxic monoxide emissions, which quickly overtake the carbon dioxide in overall amount of emission. The conclusion here is simple - it is absolutely crucial to burn this type of gas in a very lean mixture, because of the dangers mentioned.

At the end we can compare the calculated LHV of $LHV = 1,63 MJ/m_n^3$ to data from [2]



The image shows handwritten calculations in Polish. The first line is: "ciepło spalania $Q_u = 17600 + 19700 \text{ kJ}/m_n^3$ ". The second line is: "wartość opałowa $Q_L = 16000 + 17600 \text{ kJ}/m_n^3$ ".

Figure 6.1. Lower heating value

We can clearly see, that we are within the solution space.

7. References

- 1 Koksownictwo część pierwsza, Aleksander Karcz, 1991
- 2 Koksownictwo część druga, Aleksander Karcz, 1991
- 3 stackoverflow.com