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THÈME

Study and Analysis of the Thermal and Energetic Performance of Furnace F201 within the CP1/Z Complex

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Abstract

This work presents a pioneering study on the thermal and energy performance of the reforming furnace F201 in the CP1/Z petrochemical complex, integrating advanced numerical simulation with artificial intelligence (AI) techniques for the first time in this domain. The furnace, a critical unit in methanol production, operates under highly demanding thermal and chemical conditions, where optimal control is essential for both efficiency and reliability.

A theoretical model based on thermodynamic and chemical kinetics equations was developed and implemented using Python, enabling the evaluation of temperature profiles, reaction progress, and energy efficiency. Beyond classical analysis, this study introduces AI-based modeling, allowing for real-time approximation of complex nonlinear relationships between operational variables and furnace performance. The AI approach provides high-precision predictions, offering a transformative tool for monitoring, optimization, and intelligent control in industrial settings.

Highlight results the importance of thermal management, steam-to-carbon ratio, and heat recovery optimization. The hybrid methodology combining physical modeling, numerical simulation, and AI not only enhances furnace performance but also reduces fuel consumption, extends catalyst lifespan, and contributes to sustainable industrial processes. This work establishes a foundation for future applications of AI in high-temperature industrial reactors, representing a significant advancement toward intelligent and energy-efficient chemical processes.

Keywords: Reforming furnace, Methanol, Energy efficiency, Heat transfer, Simulation, Artificial Intelligence, Python

Résumé

Cette étude constitue une première approche dans l'analyse thermique et énergétique du four de reformage F201 au sein du complexe pétrochimique CP1/Z, en intégrant pour la première fois des techniques avancées de simulation numérique et d'intelligence artificielle (IA). Le four, unité essentielle de la production de méthanol, fonctionne dans des conditions thermiques et chimiques très exigeantes, nécessitant un contrôle optimal pour garantir efficacité et fiabilité.

Un modèle théorique basé sur les équations thermodynamiques et cinétiques chimiques a été développé et simulé avec Python, permettant d'évaluer les profils de température, l'avancement des réactions et l'efficacité énergétique. Au-delà de l'analyse classique, cette étude introduit une modélisation pilotée par l'IA, capable d'approximer en temps réel les relations non linéaires complexes entre les variables opérationnelles et la performance du four. Cette approche offre des prédictions précises et constitue un outil transformateur pour la surveillance, l'optimisation et le contrôle intelligent en milieu industriel.

Les résultats soulignent l'importance de la gestion thermique, du ratio vapeur/carbone et de l'optimisation de la récupération de chaleur. La méthodologie hybride combinant modélisation physique, simulation numérique et intelligence artificielle (IA) améliore la performance du four, réduit la consommation de combustible, prolonge la durée de vie des catalyseurs et contribue à la durabilité des procédés industriels. Ce travail ouvre la voie à l'utilisation de l'IA dans les réacteurs industriels à haute température et représente un progrès majeur vers des processus chimiques intelligents et économes en énergie.

Mots-clés : Four de reformage, Méthanol, Efficacité énergétique, Transfert de chaleur, Simulation, Intelligence artificielle, Python

ملخص

تقدم هذه الدراسة تجربة رائدة في تحليل الأداء الحراري والطاقوي لفرن التشكيل F201 في مجمع CP1/Z البتروكيميائي، حيث تم دمج تقنيات المحاكاة الرقمية المتقدمة مع الذكاء الاصطناعي (AI) لأول مرة في هذا المجال. يعد الفرن وحدة أساسية في إنتاج الميثانول، ويعمل في ظروف حرارية وكيميائية، مما يستلزم التحكم الأمثل لضمان الكفاءة والموثوقية.

تم تطوير نموذج نظري قائم على المعادلات الحرارية والكيميائية، وتنفيذه باستخدام Python، ما مكن من تقييم توزيع درجات الحرارة، تقدم التفاعلات، وكفاءة استهلاك الطاقة. إضافة إلى التحليل التقليدي، قدمت الدراسة نموذجًا مدفوعًا بالذكاء الاصطناعي لتقريب العلاقات غير الخطية المعقدة بين المتغيرات التشغيلية وأداء الفرن في الزمن الحقيقي. وقد أظهر هذا النهج القدرة على تقديم تنبؤات دقيقة، ما يجعله أداة مبتكرة للمراقبة، والتحسين، والتحكم الذكي في البيئات الصناعية.

أظهرت النتائج أهمية إدارة الحرارة، والحفاظ على النسبة المناسبة بين البخار والكربون، وتحسين أنظمة استرجاع الحرارة. إن المنهجية الهجينة التي تجمع بين النمذجة الفيزيائية، والمحاكاة الرقمية، والذكاء الاصطناعي تعزز أداء الفرن، وتقلل استهلاك الوقود، وتطيل عمر الحفاز، وتدعم استدامة العمليات الصناعية. يمثل هذا العمل قاعدة صلبة لتطبيق الذكاء الاصطناعي في المفاعلات الصناعية عالية الحرارة، ويشكل خطوة مهمة نحو عمليات كيميائية ذكية وموفرة للطاقة.

الكلمات المفتاحية: فرن الإصلاح، الميثانول، الكفاءة الطاقوية، انتقال الحرارة، المحاكاة، الذكاء الاصطناعي، Python

Dedication

إهداء

وَقُل رَّبِّ زِدْنِي عِلْمًا

(سورة طه، آية 114)

أهدي هذا العمل إلى أمي الحبيبة، رمز الحب والصبر، وإلى أبي العزيز، مصدر الدعم والتشجيع، على كل ما قدموه لي من رعاية، حب، وتوجيه طوال حياتي الدراسية والعلمية.

شكراً لكم من القلب على صبركم وثقتكم بي، هذا الإنجاز هو ثمرة دعائكم وتشجيعكم الدائم.

هويدف محمد

إهداء

قال رسول الله صلى الله عليه وسلم: "من سلك طريقًا يلتمس فيه علمًا سهل الله له به طريقًا إلى الجنة"

(رواه مسلم)

أهدي هذا العمل إلى زميلي العزيز، رفيق الدرب في هذه المرحلة الدراسية، الذي شاركني الجهد والتعب، وكان سندًا وداعمًا لي في مختلف مراحل إنجاز هذا العمل.

كما أهديه إلى والديا الكريمين، اللذين كان لهما الفضل في دعمي وتشجيعي، وغرس قيم الاجتهاد والمثابرة في نفسي.

شكراً لكم على ما قدمتموه من دعم وثقة، فهذا الإنجاز هو ثمرة دعائكم المستمر.

قدور غداوي عبد الكريم

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First and foremost, I would like to thank Allah for giving me the strength and patience to complete this work.

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General Introduction

In the context of the continuously increasing global energy demand and the growing environmental challenges associated with greenhouse gas emissions, improving the efficiency of industrial energy systems has become a major priority in modern engineering. Today, industrial performance is no longer evaluated solely on production capacity, but also on energy efficiency, operational optimization, and environmental impact, in line with sustainable development objectives.

Within this framework, the petrochemical industry plays a crucial role, as it is one of the most energy-intensive sectors. Among its key processing units, steam reforming furnaces represent a central component, particularly in methanol production. Furnace F201, operating within the CP1/Z complex, is responsible for converting natural gas into synthesis gas (syngas), a mixture rich in hydrogen, through highly endothermic chemical reactions that require elevated temperatures and substantial heat input.

Despite its industrial importance, the operation of Furnace F201 presents several technical challenges. These include high energy consumption, significant thermal losses, and operational issues such as coke formation and catalyst deactivation. These factors directly affect the efficiency, reliability, and lifetime of the furnace, making its thermal and energy analysis essential for performance improvement.

Traditionally, such systems are analyzed using physical and mathematical models based on heat transfer principles and chemical reaction kinetics. While these models provide a deep understanding of the underlying phenomena, they are often complex and computationally demanding, especially when dealing with nonlinear, multi-variable systems like reforming furnaces.

In recent years, artificial intelligence (AI) and deep learning techniques have increasingly emerged as powerful tools for modeling and optimizing complex industrial processes. Unlike conventional approaches, AI models are capable of learning nonlinear relationships directly from data, without explicitly solving differential equations. This enables fast prediction, adaptive control, and real-time optimization of process performance, representing a significant advancement in process engineering.

In this context, the present work aims to study and analyze the thermal and energy performance of Furnace F201 within the CP1/Z complex by adopting an integrated approach. This approach combines theoretical modeling, numerical simulation using Python

[1], and the exploration of artificial intelligence techniques for performance prediction and optimization.

Furthermore, a comparison between theoretical results and simulated or real operational data is carried out to evaluate furnace efficiency, identify sources of energy losses, and propose practical solutions for improvement. This study seeks to provide a deeper understanding of furnace behavior and to introduce modern tools that support engineers in making more efficient and informed decisions.

Finally, this work aligns with the global trend toward industrial digitalization and the development of intelligent energy systems. By integrating classical engineering principles with data-driven approaches, it contributes to enhancing energy efficiency, reducing operational costs, and supporting the transition toward more sustainable industrial processes.

Chapter 1

General Presentation of SONATRACH and the Petrochemical Complex (CP1/Z)

1.1 Introduction

This chapter provides a general overview of Sonatrach and the petrochemical complex CP1/Z. It also introduces natural gas and the methanol production process.

Figure 1.1: Sonatrach Corporation.
[2]

1.2 Overview of SONATRACH

SONATRACH is the national oil and gas company of Algeria and is considered the largest company in Africa and a major player in the global energy sector[3]. It was established

on December 31, 1963, following Algeria's independence, as a fully state-owned company with the mission to manage, develop, and preserve the country's vast hydrocarbon resources. Over the decades, Sonatrach has grown to become a fully integrated energy company involved in all aspects of the petroleum value chain, from upstream exploration to downstream marketing.

Historical Background:

The establishment of Sonatrach came at a critical period for Algeria's newly independent economy. Initially, foreign companies controlled most of the hydrocarbon sector. By nationalizing the oil and gas industry, Algeria aimed to assert sovereignty over its resources and generate national revenue. Sonatrach gradually expanded its capabilities through joint ventures and partnerships with international companies, acquiring modern technologies and expertise in exploration, extraction, and processing.

Organizational Structure:

Sonatrach operates under the supervision of the Ministry of Energy and Mines. The company is organized into several subsidiaries and branches, each responsible for specific activities such as exploration, production, pipelines, petrochemicals, and commercial distribution. It has a structured hierarchy including a Board of Directors, a CEO, and specialized technical departments to manage operations across Algeria and internationally.

Main Activities:

Sonatrach's operations are comprehensive and cover the entire hydrocarbon chain:

- **Exploration:** Sonatrach conducts geological surveys, seismic studies, and exploratory drilling to locate new oil and gas fields within Algeria's territory, both onshore and offshore.
- **Extraction:** The company operates numerous oil fields and gas fields, utilizing advanced drilling technologies to optimize production and efficiency.
- **Transportation:** Sonatrach manages an extensive network of pipelines for crude oil and natural gas, ensuring secure delivery to domestic refineries and export terminals.
- **Refining and Processing:** Through its refineries, Sonatrach converts crude oil into refined products such as gasoline, diesel, and jet fuel, while also producing petrochemical feedstocks.
- **Gas Liquefaction and Export:** Sonatrach operates liquefied natural gas (LNG) plants, enabling Algeria to export gas to Europe and other global markets.
- **Marketing and Commercial Distribution:** The company handles domestic and international sales of petroleum products, maintaining a strong presence in both Algerian and foreign markets.

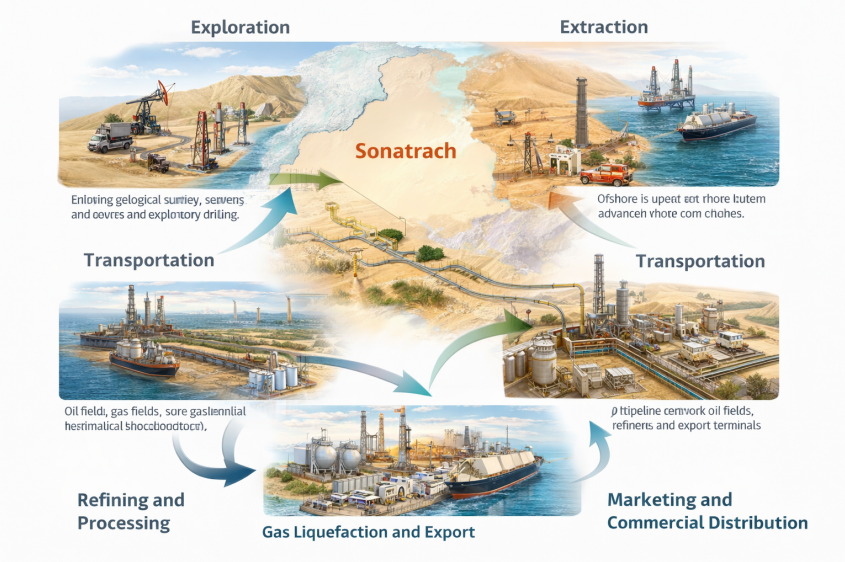

Figure 1.2: Sonatrach's operational cycle.

Economic and Strategic Importance:
Sonatrach is crucial for Algeria's economy, providing a significant portion of national revenue, foreign exchange earnings, and employment. Its exports, particularly natural gas to Europe, make it a strategic player in the regional energy market. The company also contributes to technological development and local industry through partnerships, training programs, and investment in energy infrastructure.

International Presence:
In addition to domestic operations, Sonatrach has international activities, including joint ventures with global energy firms and participation in exploration and production projects abroad. These initiatives enhance Algeria's global energy influence and bring in foreign investment and advanced technologies.

Research and Innovation:
Sonatrach invests in research centers and technical training institutes to advance the hydrocarbon sector, develop sustainable extraction techniques, and optimize refinery and LNG operations. Innovation is central to its strategy for maintaining competitiveness in the global market.

With more than 50 years of experience, Sonatrach has transformed Algeria into a major oil and gas producer and exporter. Its integrated operations, international partnerships, and strategic vision ensure the company remains a pillar of Algeria's economy and a key player in global energy markets.

1.3 Presentation of the CP1/Z Complex

1.3.1 Historical Background

The CP1/Z complex was established in 1969 as a result of a strategic partnership between Sonatrach and an Italian engineering firm. This collaboration aimed to develop Algeria's petrochemical industry and to utilize the country's abundant natural gas resources efficiently. Over the years, the complex has undergone expansions and modernization programs to increase capacity, improve safety standards, and incorporate new technologies [8].

Key historical milestones:

- **1970: Launch of the project in Arzew** – Initial construction work began, including site preparation, basic infrastructure, and installation of utility systems.
- **1971: Contract for methanol unit** – Technical design and supply contracts were signed for the methanol production unit, marking the start of Algeria's first large-scale methanol production.
- **1975: Start of utility units** – Essential support systems, including steam generation, water treatment, and power supply, were commissioned to ensure continuous operations.
- **1976: Methanol production start** – The methanol unit began producing methanol at commercial scale, using natural gas as the main feedstock.
- **1977: Resin production start** – Production of synthetic resins, including formaldehyde-based resins and urea-formaldehyde resins, was initiated to supply domestic and export markets.

1.3.2 Location

The CP1/Z complex is strategically located in the Arzew industrial zone in the Oran province of Algeria. The site was selected based on proximity to natural gas pipelines, the port of Arzew for exports, and the road network connecting Oran and Mostaganem.

Figure 1.3: Location of CP1/Z complex. [7]

- **Area:** The site covers approximately 27 hectares, providing sufficient space for current facilities and future expansions.
- **Proximity:** Only 2 km from Arzew city, facilitating logistics, workforce accessibility, and administrative coordination.
- **Connectivity:** Adjacent to the Oran–Arzew–Mostaganem highway, enhancing transportation of products and raw materials.

1.3.3 Objectives

The CP1/Z complex was designed to achieve multiple strategic objectives:

- **Natural gas processing:** Transform raw natural gas into valuable feedstocks for chemical production.
- **Petrochemical production:** Manufacture methanol and synthetic resins for industrial and commercial use.
- **Supply of national market:** Ensure consistent delivery of chemical products to Algerian industries.
- **Export:** Contribute to national revenue by supplying methanol and resins to international markets.

1.3.4 Products

- **Methanol:** High-purity methanol used for industrial applications, chemical synthesis, and fuel additives.
- **Synthetic resins:** Includes multiple resin types:
  - **Formaldehyde 36%** – Used in adhesives and construction materials.
  - **Formir 80%** – High-performance resin for industrial applications.
  - **Urea resins** – Employed in laminates, wood adhesives, and coatings.

1.4 Natural Gas

1.4.1 Definition

Natural gas is a fossil fuel predominantly composed of methane. It is formed over millions of years through the decomposition of organic matter under heat and pressure in geological formations. As a clean and versatile energy source, it is essential for power generation, heating, and chemical production, including methanol synthesis.

1.4.2 Composition

- **Methane (CH_4):** 81%--97%, the primary component responsible for energy content.
- **Ethane (C_2H_6):** Minor component, used as a petrochemical feedstock.
- **Propane (C_3H_8):** Used in heating, transportation, and chemical processes.
- **Butane (C_4H_{10}):** Also used as fuel and in petrochemical applications.

1.5 Methanol Production Process

The production of methanol at the CP1/Z complex is carried out through a sophisticated multi-unit process that transforms natural gas, primarily composed of methane, into methanol. This conversion relies on a sequence of carefully controlled chemical reactions facilitated by advanced catalytic technologies. Initially, natural gas undergoes a pretreatment phase to remove impurities such as sulfur compounds, which could poison the catalysts used in subsequent steps. Following this, the purified gas enters the reforming unit, where it reacts with steam in the presence of a catalyst to produce synthesis gas, a mixture of hydrogen, carbon monoxide, and carbon dioxide.

The synthesis gas is then cooled and adjusted in composition to achieve the optimal H_2/CO ratio for methanol synthesis. This mixture is fed into the methanol reactor, where catalytic reactions convert it into methanol under high pressure and temperature conditions. The resulting crude methanol undergoes a series of purification steps, including distillation and separation, to remove water and by-products, yielding high-purity methanol ready for industrial applications.

Overall, the CP1/Z process combines modern engineering design with effective operational strategies to enhance production yield, improve energy efficiency [5], and reduce environmental impact. Furthermore, every unit in the process, including the reformer, reactor, and separation columns, contributes significantly to maintaining continuous and efficient methanol production.

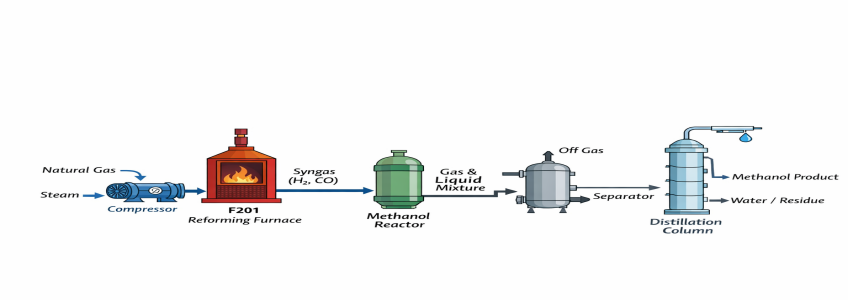

Figure 1.4: Process Flow Diagram of Methanol Production via Furnace F201.

- **Unit 100: Gas distribution** – Natural gas is received at 30 bar, measured, and routed to various process lines including fuel gas, process gas, and protective gas circuits.
- **Unit 200: Reforming furnace** – Gas is mixed with steam and passed over a nickel-based catalyst at high temperature to produce synthesis gas (a mixture of CO and H_2).
- **Unit 300: Cooling** – The hot synthesis gas is cooled to approximately 40°C, and condensed water is removed to prevent downstream corrosion.
- **Unit 400: Compression** – Synthesis gas is compressed from 17.5 bar to 50 bar to achieve the conditions necessary for the methanol synthesis reactor.
- **Unit 500: Reactor** – Methanol is synthesized using a copper-based catalyst in a high-pressure reactor under controlled temperature and pressure.
- **Unit 600: Distillation** – Crude methanol is purified through two distillation columns to achieve the required product specifications.
- **Unit 700: Steam generation** – Steam is produced to operate turbines, pumps, and other auxiliary equipment throughout the complex.

1.6 Process Description

1.6.1 Unit 100 – Gas Distribution

This unit ensures the precise allocation of natural gas to all sections of the plant. Safety valves, flow meters, and regulators are installed to monitor pressure and flow, guaranteeing continuous and safe operation, as illustrated in Figure 1.5.

Figure 1.5: Process Flow Diagram of Unit 100 – Gas Distribution System.

1.6.2 Unit 200 – Reforming Furnace

Natural gas is reformed with steam at high temperatures over a nickel catalyst. This endothermic reaction generates a synthesis gas mixture, which is the essential precursor for methanol production, as shown in Figure 1.6.

Figure 1.6: Reforming Furnace in Unit 200.

1.6.3 Unit 300 – Cooling and Water Removal

As illustrated in Figure 1.7,the synthesis gas is cooled using heat exchangers to approximately 40°C. Condensed water is separated to protect downstream equipment, prevent corrosion, and improve catalyst efficiency.

(a) P.Overview of U.300 – Cooling and Water Removal.

(b) Front View of the Heat Exchanger.

(c) Side View of the Heat Exchanger.

Figure 1.7: Unit 300 – Cooling and Water Removal System: Heat Exchanger and Water Separation.

1.6.4 Unit 400 – Compression

The cooled synthesis gas is compressed to 50 bar. This high-pressure gas is required to drive the methanol synthesis reaction to achieve high conversion rates in the reactor Figure 1.8.

Figure 1.8: Unit 400: Compression.

1.6.5 Unit 500 – Methanol Reactor

Synthesis gas is fed into a reactor containing a copper-based catalyst (Figure 1.9). Methanol is produced via the reaction between CO and H_2 under controlled temperature and pressure. Continuous monitoring ensures high product yield and quality.

Figure 1.9: Process Flow Diagram of Unit 500 – Methanol Reactor.

1.6.6 Unit 600 – Distillation

The crude methanol mixture undergoes purification in two consecutive distillation columns (Figure 1.10). This step removes water and by-products, delivering methanol that meets industrial and commercial specifications.

Figure 1.10: Unit 600 – Distillation.

1.6.7 Unit 700 – Steam Generation

Steam is generated to provide energy for turbines, pumps, and heat exchangers (Figure 1.11), supporting both the methanol production process and auxiliary operations. Efficient energy management in this unit is crucial for the overall plant performance.

Figure 1.11: Steam Generation Unit.

1.7 Internship Experience and Thermal-Energetic Performance of Furnace F201

During my internship at the CP1/Z complex, I gained extensive practical experience in the petrochemical sector, with a particular focus on the methanol production units. My main attention was on Furnace F201, which plays a central role in converting natural gas into synthesis gas (syngas) for methanol production. This experience allowed me to connect theoretical knowledge of thermal processes to real industrial operations.

1.7.1 Daily Professional Activities

My daily activities consisted of going through different units to observe and assist in the operation of each unit. I learned to monitor furnace parameters, including temperature profiles, fuel consumption, and pressure, and to understand the influence of these parameters on catalyst efficiency. I also gained hands-on experience with the plant's SCADA system, recording real-time data and analyzing the furnace's thermal and energetic performance.

1.7.2 Interaction with Technical Teams

I worked closely with engineers and technicians responsible for operation and maintenance. This collaboration taught me the importance of coordination between different teams to ensure continuous operation and maintain high thermal efficiency. Maintenance activities such as inspecting piping, checking catalyst performance, and adjusting ventilation and cooling systems were key to maintaining optimal furnace performance.

1.7.3 Skills and Knowledge Acquired

Through this internship, I developed several technical skills:

- **Thermal and energetic monitoring:** Recording temperature and energy consumption data and analyzing efficiency.
- **Process control:** Using SCADA and digital control panels to monitor furnace operations.
- **Maintenance awareness:** Understanding the impact of routine maintenance on thermal performance and energy efficiency.
- **Problem-solving and teamwork:** Collaborating with engineers and technicians to identify and correct deviations in furnace performance.

- **Safety compliance:** Following industrial safety protocols in high-temperature and high-pressure environments.

Figure 1.12: Skills and Knowledge Acquired.

1.7.4 Operational Data Collection

To analyze the thermal and energetic performance of Furnace F201, I created a monitoring table to record key parameters. This table provides systematic tracking of furnace performance and identifies areas for improvement.

Table 1.1: Temperature, pressure, and concentration measurements.

No.	T_{in} ($^{\circ}C$)	T_{out} ($^{\circ}C$)	Pressure (bar)	Concentration (Nm^3/h)
1	400	730	19.0	11500
2	409	760	19.2	12100
3	402	731	19.1	11730
4	401	738	19.2	11520
5	400	741	18.9	11582
6	401	738	19.3	11552
7	405	745	19.1	11535

1.7.5 Column Explanation

- **Inlet Temp (°C):** Temperature of natural gas entering the furnace.
- **Outlet Temp (°C):** Temperature of synthesis gas leaving the furnace before cooling.

- **Steam Pressure (bar):** Pressure of steam used for the gas-steam reaction.
- **Gas Consumption (Nm^3/h):** Volume of natural gas consumed per hour.

1.7.6 Performance Analysis and Recommendations

Based on collected data and observations, several recommendations can improve thermal and energetic efficiency:

- Optimize the gas and steam flow rates to maintain uniform temperature distribution.
- Inspect and improve thermal insulation to minimize heat losses.
- Implement regular catalyst maintenance to sustain high conversion rates.
- Utilize additional temperature sensors to monitor the furnace more precisely.
- Develop a simulation model [1] to predict furnace behavior under varying operational conditions.
- Maintain a detailed maintenance schedule focusing on critical components.

1.7.7 Schematic of Heat and Energy Flow

The furnace's thermal and energetic flow can be represented as follows:

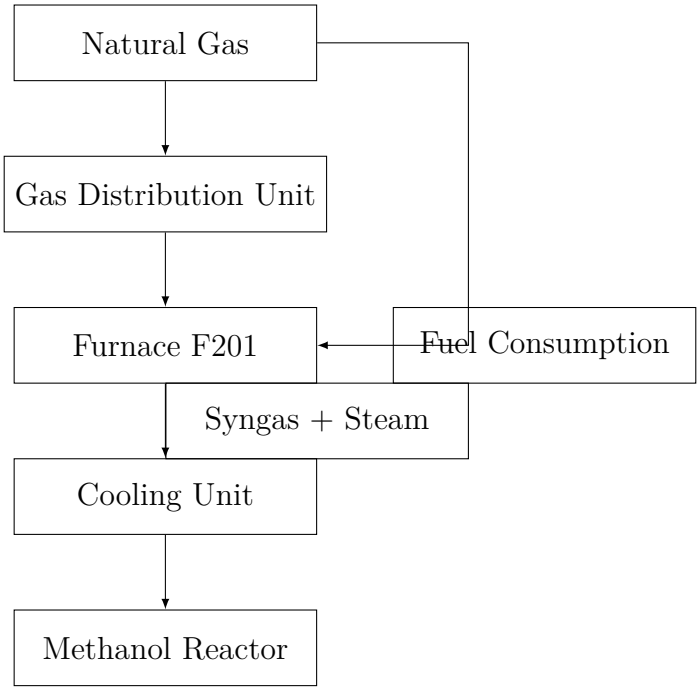

Figure 1.13: Simplified Process Flow Diagram of Methanol Production.

1.8 Conclusion

This chapter has provided a comprehensive overview of the CP1/Z complex, detailing its historical development, strategic objectives, location, products, and the technical aspects of the methanol production process. The detailed description of each unit highlights the complexity and integration of operations necessary to transform natural gas into high-quality methanol and synthetic resins.

Furthermore, this internship provided an in-depth understanding of Furnace F201's thermal and energetic performance. By monitoring operational parameters, analyzing energy consumption, and observing industrial processes firsthand, I acquired both practical and analytical skills that will be instrumental for my study entitled ``Étude et analyse des performances thermiques et énergétiques du four F201 au sein du complexe CP1/Z''.

The combination of data collection, performance monitoring, and improvement recommendations provides a solid basis for evaluating and optimizing furnace efficiency in an industrial context. Overall, this work establishes a strong foundation for understanding the operational behavior of Furnace F201 and contributes to improving the overall efficiency and reliability of the methanol production process within the CP1/Z complex.

Chapter 2

Thermal and Energy Analysis of Furnace F201

2.1 Introduction

Furnace F201 plays a central role in the methanol production process at the CP1/Z complex, where it is responsible for converting natural gas into synthesis gas (syngas), a mixture primarily composed of hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2). This transformation is achieved through high-temperature catalytic reactions, mainly steam methane reforming reaction (SMR) [4].

Due to the highly endothermic nature of the reforming reactions, the furnace requires a continuous and well-controlled heat supply. Consequently, Furnace F201 is not only a chemical reactor but also a complex thermal system where combustion, heat transfer, and reaction kinetics interact simultaneously.

The performance of this furnace has a direct impact on:

- Hydrogen production yield
- Fuel consumption
- Catalyst lifetime
- Overall plant efficiency

For these reasons, a detailed thermal and energy analysis is essential to understand its behavior and optimize its operation. This chapter presents a comprehensive study combining theoretical modeling, thermodynamic analysis, and numerical simulation using Python tools.

2.2 Thermal Analysis

2.2.1 Main Chemical Reactions

The operation of Furnace F201 is governed by two main reactions:

Steam Methane Reforming (SMR):

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \quad \Delta H^\circ = +206\,\text{kJ/mol} \tag{2.1}$$

This reaction is strongly endothermic and requires continuous heat input.

Water-Gas Shift Reaction (WGS):

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \Delta H^\circ = -41\,\text{kJ/mol} \tag{2.2}$$

This reaction enhances hydrogen production.

2.2.2 Side Reactions and Coke Formation

Undesired reactions lead to coke formation:

$$CH_4 \rightarrow C + 2H_2 \tag{2.3}$$

$$2CO \rightarrow C + CO_2 \tag{2.4}$$

Coke deposition reduces catalyst activity and blocks heat transfer. It is mainly influenced by temperature distribution and the steam-to-carbon ratio.

2.2.3 Heat Transfer Mechanisms

Heat transfer in furnaces occurs through three main mechanisms: radiation, convection, and conduction. Radiation becomes the dominant heat transfer mode at high temperatures, where heat is transferred in the form of electromagnetic waves without requiring a medium. Convection involves the transfer of heat due to the motion of fluids such as hot gases, while conduction refers to heat transfer through solid materials as a result of temperature gradients. Heat transfer occurs through:

- Radiation (dominant)
- Convection
- Conduction

$$Q = U \cdot A \cdot (T_{furnace} - T_{gas}) \tag{2.5}$$

Where:

- Q: Heat transfer rate (W)
- U: Overall heat transfer coefficient (W/m^2·K), represents the efficiency of heat transfer across all thermal resistances
- A: Heat transfer surface area (m^2)
- $T_{furnace}$: Furnace temperature (K or °C)
- T_{gas}: Gas temperature inside the tube (K or °C)
- $(T_{furnace} - T_{gas})$: Temperature difference (driving force for heat transfer)

2.2.4 Energy Balance in the Tube

The energy balance along the reactor tube describes how heat is transferred and consumed as the process fluid flows through the system. As the fluid moves in the axial direction (z), its temperature changes due to two main effects: the heat added or removed from the surroundings, and the heat generated or absorbed by chemical reactions occurring inside the tube. This balance is essential for predicting temperature profiles and ensuring safe and efficient reactor operation.

The energy balance can be expressed as:

$$\frac{dQ}{dz} = \dot{m} C_p \frac{dT}{dz} + \sum r_i \Delta H_i \tag{2.6}$$

Where:

- $\frac{dQ}{dz}$: Heat transfer rate per unit length of the tube (W/m), representing the amount of heat added to or removed from the fluid along the reactor
- $\dot{m}$: Mass flow rate of the fluid (kg/s), indicating how much mass passes through the tube per unit time
- C_p: Heat capacity at constant pressure (J/kg·K), which measures the amount of energy required to raise the temperature of the fluid
- $\frac{dT}{dz}$: Temperature gradient along the tube (K/m), describing how the fluid temperature changes with respect to the axial position
- $\sum r_i \Delta H_i$: Heat effect of chemical reactions (W/m), where:

– r_i: Reaction rate of component i (mol/m^3·s)
– ΔH_i: Enthalpy change of reaction i (J/mol), negative for exothermic reactions (heat released) and positive for endothermic reactions (heat absorbed)

This equation shows that the heat supplied to the system is used partly to increase the temperature of the flowing fluid (sensible heat) and partly to drive chemical reactions (reaction heat).

2.2.5 Steam-to-Carbon Ratio

The steam-to-carbon ratio (S/C) is a key operating parameter in steam reforming processes, especially in methane reforming. It represents the amount of steam fed relative to the carbon-containing feed (typically methane). This ratio strongly influences reactor performance, catalyst stability, and the extent of side reactions such as coke formation.

The ratio is defined as:

$$S/C = \frac{F_{H_2O}}{F_{CH_4}} \tag{2.7}$$

Where:

- S/C: Steam-to-carbon ratio (dimensionless), indicates the proportion of steam relative to carbon in the feed
- F_{H_2O}: Molar flow rate of steam (mol/s), representing the amount of water vapor entering the reactor
- F_{CH_4}: Molar flow rate of methane (mol/s), representing the carbon source in the feed

A higher S/C ratio means that more steam is present relative to methane. This has several important effects:

- It reduces the formation of coke (solid carbon) on the catalyst surface. Coke forms through side reactions such as methane cracking or the Boudouard reaction, and it can deactivate the catalyst by blocking active sites.
- It shifts the chemical equilibrium toward hydrogen production, improving the yield of hydrogen in reforming reactions.
- However, increasing the steam content requires more energy, since additional heat is needed to generate and superheat the steam. This leads to higher operational costs and energy consumption.

Therefore, the S/C ratio must be carefully optimized to balance between minimizing coke formation and maintaining reasonable energy efficiency.

2.2.6 Thermal Constraints

Typical outlet temperature: $\approx 850°C$

- High temperature $\rightarrow$ tube damage
- Low temperature $\rightarrow$ incomplete conversion

2.2.7 Thermal Analysis Discussion

The furnace operates under a delicate balance between heat supply and reaction demand. Any imbalance leads either to energy losses or reduced conversion efficiency. Coke formation remains one of the most critical challenges, directly linked to temperature gradients and insufficient steam.

2.3 Energy Analysis

2.3.1 Global Energy Balance

The global energy balance represents the overall distribution of energy in the furnace or process unit. It states that the total heat released by fuel combustion is divided into two main parts: the useful heat transferred to the process, and the heat lost to the surroundings. This equation is essential for evaluating thermal efficiency and identifying where energy losses occur in the system.

The global energy balance can be written as:

$$Q_{\text{fuel}} = Q_{\text{process}} + Q_{\text{losses}} \tag{2.8}$$

Where:

- Q_{fuel}: Total heat supplied by fuel combustion (W or kW), representing the energy generated by burning the fuel in the furnace
- Q_{process}: Useful heat absorbed by the process (W or kW), including the energy required to heat the reactants, raise the gas temperature, and support endothermic reactions
- Q_{losses}: Heat losses to the surroundings (W or kW), including losses through furnace walls, radiation to the environment, and hot flue gases leaving the system

This equation shows that not all of the energy released by the fuel is effectively used by the process. A portion is always lost, and minimizing these losses is important for improving furnace efficiency, reducing fuel consumption, and lowering operating costs.

2.3.2 Fuel Energy Input

The fuel energy input represents the total amount of thermal energy supplied to the system through fuel combustion. This energy is the primary source driving the heating process inside the furnace and enabling endothermic reactions. It depends on both the amount of fuel burned and its heating value.

$$Q_{\text{fuel}} = \dot{m}_{\text{fuel}} \cdot LHV \tag{2.9}$$

Where:

- Q_{fuel}: Total heat input from fuel (W or kW)
- $\dot{m}_{\text{fuel}}$: Mass flow rate of fuel (kg/s)
- LHV: Lower Heating Value (J/kg), representing the usable energy released during combustion excluding latent heat of vaporization

2.3.3 Useful Heat

Useful heat is the portion of energy that is effectively utilized by the process. It includes both the heat required to raise the temperature of the fluid (sensible heat) and the heat consumed or released by chemical reactions.

$$Q_{\text{process}} = Q_{\text{sensible}} + Q_{\text{reaction}} \tag{2.10}$$

Where:

- Q_{process}: Total useful heat absorbed by the process
- Q_{sensible}: Heat used to increase fluid temperature
- Q_{reaction}: Heat associated with chemical reactions (positive for endothermic, negative for exothermic)

The sensible heat can be calculated as:

$$Q_{\text{sensible}} = \dot{m} C_p (T_{out} - T_{in}) \tag{2.11}$$

Where:

- $\dot{m}$: Mass flow rate of the process fluid (kg/s)
- C_p: Heat capacity (J/kg·K)
- T_{out}: Outlet temperature (K or °C)

- T_{in}: Inlet temperature (K or °C)
- $(T_{out} - T_{in})$: Temperature rise of the fluid

2.3.4 Heat Losses

Heat losses represent the portion of energy that is not utilized by the process and is lost to the surroundings. These losses reduce the overall efficiency of the system.

- Flue gas losses: Heat carried away by hot exhaust gases leaving the furnace
- Radiation losses: Heat lost through furnace walls by thermal radiation
- Incomplete combustion: Energy lost due to unburned fuel or partial combustion

The heat loss due to flue gas can be estimated by:

$$Q_{\text{flue}} = \dot{m}_{\text{flue}} C_p (T_{\text{flue}} - T_{\text{ambient}}) \tag{2.12}$$

Where:

- Q_{flue}: Heat loss with flue gases (W or kW)
- $\dot{m}_{\text{flue}}$: Mass flow rate of flue gas (kg/s)
- C_p: Heat capacity of flue gas (J/kg·K)
- T_{flue}: Flue gas temperature (K or °C)
- T_{ambient}: Ambient temperature (K or °C)

2.3.5 Furnace Efficiency

Furnace efficiency expresses how effectively the energy from fuel is converted into useful heat for the process. A higher efficiency indicates better utilization of fuel energy and lower losses.

$$\eta = \frac{Q_{\text{process}}}{Q_{\text{fuel}}} \tag{2.13}$$

Where:

- η: Furnace efficiency (dimensionless or %)
- Q_{process}: Useful heat absorbed by the process
- Q_{fuel}: Total heat supplied by fuel

2.3.6 Exergy Analysis

Exergy analysis evaluates the quality of energy and its ability to perform useful work. Unlike energy, exergy accounts for irreversibilities and losses due to entropy generation. It is particularly useful for identifying inefficiencies in thermal systems.

$$Ex = Q\left(1 - \frac{T_0}{T}\right) \tag{2.14}$$

Where:

- Ex: Exergy associated with heat transfer (W)
- Q: Heat transfer (W)
- T: Temperature at which heat is supplied (K)
- T_0: Ambient (reference) temperature (K)
- $\left(1 - \frac{T_0}{T}\right)$: Exergy factor, representing the fraction of heat that can be converted into useful work

This analysis helps identify where useful energy is degraded and provides deeper insight than energy balance alone.

2.3.7 Energy Analysis Discussion

The main source of inefficiency in Furnace F201 is the loss of high-temperature energy through exhaust gases. Improving insulation and heat recovery systems can significantly enhance performance. Additionally, optimizing combustion conditions reduces fuel consumption and improves thermal efficiency.

2.4 Mathematical Modeling and Simulation

Mathematical modeling and simulation have become fundamental tools in engineering and scientific research, particularly in the field of chemical and thermal processes. At their core, these approaches allow engineers and researchers to represent complex physical, chemical, and thermal systems using mathematical equations and computational algorithms. By abstracting real-world phenomena into a formalized model, one can predict system behavior, optimize performance, and test different operational scenarios without the cost and risk of conducting extensive physical experiments.

Mathematical Modeling: Mathematical modeling involves the formulation of equations that describe the relationships between the variables of a system. These equations can be algebraic, differential, or even stochastic, depending on the complexity and nature

of the process being studied. In chemical engineering, for instance, models often represent mass balances, energy balances, reaction kinetics, and transport phenomena. The primary goal is to create a framework that captures the essential dynamics of the system, providing insight into how inputs, environmental conditions, and operational parameters affect outputs. Models can range from simple idealized representations to highly detailed mechanistic models that incorporate multiple coupled phenomena.

Simulation: Once a model is established, simulation enable one to numerically solve the equations under various conditions. Simulation provides a virtual laboratory where engineers can explore the impact of changes in parameters such as temperature, pressure, flow rates, and chemical composition. This is particularly useful in industrial contexts, where experimenting directly on large-scale equipment can be expensive, dangerous, or impractical. Simulation results can reveal potential inefficiencies, predict critical operating conditions, and support decision-making for system design, control, and optimization.

Role of Python: In recent years, Python [6] has emerged as one of the most popular programming languages for modeling and simulation, due to its simplicity, flexibility, and the extensive ecosystem of scientific libraries. Libraries such as `NumPy`, `SciPy`, and `Pandas` provide powerful tools for numerical computation and data manipulation, while `Matplotlib` and `Seaborn` facilitate visualization of simulation results. For more advanced modeling, frameworks like `SimPy` and `Pyomo` enable simulation of dynamic systems and optimization problems. In the context of chemical process modeling, Python allows researchers to implement complex differential equations representing reaction kinetics, heat and mass transfer, and energy balances, then solve them efficiently to analyze system behavior under varying operational scenarios.

Application to Furnace F201: The reforming furnace F201 in the CP1/Z petrochemical complex presents a highly nonlinear and thermally demanding system. The conversion of natural gas into synthesis gas via steam methane reforming involves endothermic reactions that require precise thermal management to maintain catalyst activity and avoid material degradation. Developing a mathematical model of Furnace F201 involves defining energy balances along the reformer tubes, modeling the kinetics of the reforming reaction, and including heat transfer mechanisms such as conduction, convection, and radiation from the burners. Once the model is formulated, Python-based simulations allow the study of temperature profiles, methane conversion, and efficiency variations under different operating conditions. This enables engineers to test different scenarios, such as changing the steam-to-carbon ratio or adjusting fuel input, without any risk to the actual industrial equipment.

Integration with Artificial Intelligence: Beyond classical simulation, Python provides a convenient platform to integrate data-driven approaches, including artificial intelligence (AI) and machine learning (ML), into the modeling process. By training neural

networks on operational data, it is possible to approximate complex nonlinear relationships between input variables and performance indicators, predicting system behavior in real-time. In the case of Furnace F201, this approach can support dynamic control strategies, optimize energy consumption, and provide early warnings for abnormal operating conditions. The combination of mechanistic models with AI-enhanced simulation constitutes a hybrid methodology that leverages the predictive power of physical laws and the adaptability of data-driven techniques.

In conclusion, mathematical modeling and simulation are indispensable for understanding and optimizing industrial processes, particularly in high-temperature, energy-intensive systems such as reforming furnaces. Python serves as a versatile tool that enables both traditional numerical simulation and the integration of advanced AI methods, providing engineers with the means to enhance performance, reduce energy consumption, and ensure safe and efficient operation. In the context of Furnace F201, this methodology provide for a detailed analysis of thermal behavior, reaction kinetics, and operational efficiency, paving the way for intelligent control and sustainable process optimization.

2.4.1 Model Assumptions

- Steady-state
- One-dimensional flow
- Ideal gas
- Uniform catalyst

2.4.2 Mass Balance

$$\frac{dF_{CH_4}}{dz} = -r_{SMR} \tag{2.15}$$

2.4.3 Energy Balance

$$\frac{dT}{dz} = \frac{Q_{\text{transfer}} - \sum r_i \Delta H_i}{\dot{m} C_p} \tag{2.16}$$

2.4.4 Coke Model

$$r_{\text{coke}} = k_c \cdot C_{CH_4} \cdot \left(\frac{1}{S/C} \right) \tag{2.17}$$

2.5 Python Simulation

To complement the theoretical analysis, a simplified Python model is used to evaluate furnace efficiency.

```
import numpy as np

m_dot = 2.5
cp = 2.1
T_in = 450
T_out = 820
Q_in = 12000

Q_absorbed = m_dot * cp * (T_out - T_in)
efficiency = (Q_absorbed / Q_in) * 100

print("Efficiency:", efficiency)
```

2.5.1 Code Explanation

This program calculates the thermal efficiency of the furnace:

- **m_dot**: gas flow rate
- **cp**: heat capacity
- **T_in, T_out**: temperatures
- **Q_absorbed**: useful heat
- **efficiency**: performance indicator

The model provide testing different operating conditions quickly.

2.5.2 Simulation Discussion

The simulation demonstrates that:

- Increasing temperature improves efficiency
- Higher flow rate increases absorbed energy
- Poor heat input reduces performance

2.6 Detailed Numerical Modeling of Chemical Reactions and Heat Transfer in Furnace F201 Using Python

In order to achieve a deeper understanding of the physical and chemical phenomena occurring inside Furnace F201, a detailed numerical model is developed. Unlike simplified energy balance approaches, this model considers the coupled effects of reaction kinetics, mass transfer, and heat transfer along the reformer tubes.

2.6.1 Model Description

The reformer tube is modeled as a one-dimensional plug flow reactor (PFR), where chemical reactions and heat transfer occur simultaneously along the axial direction.

The model accounts for:

- Multiple chemical reactions (SMR, WGS, side reactions)
- Temperature variation along the tube
- Species concentration profiles
- Coke formation tendency

2.6.2 Reaction Kinetics

The main reaction rates are expressed as:

$$r_{SMR} = k_1 \exp\left(-\frac{E_1}{RT}\right) C_{CH_4} C_{H_2O} \tag{2.18}$$

$$r_{WGS} = k_2 \exp\left(-\frac{E_2}{RT}\right) C_{CO} C_{H_2O} \tag{2.19}$$

2.6.3 Mass Balance Equations

$$\frac{dC_{CH_4}}{dz} = -r_{SMR} - r_{decomp} \tag{2.20}$$

$$\frac{dC_{H_2}}{dz} = 3r_{SMR} + r_{WGS} + 2r_{decomp} \tag{2.21}$$

$$\frac{dC_{CO}}{dz} = r_{SMR} - r_{WGS} \tag{2.22}$$

2.6.4 Energy Balance Equation

$$\frac{dT}{dz} = \frac{Q_{\text{ext}} - \sum r_i \Delta H_i}{\dot{m} C_p} \tag{2.23}$$

2.6.5 Coke Formation Model

$$r_{\text{coke}} = k_c \cdot C_{CH_4} + k_b \cdot C_{CO}^2 \tag{2.24}$$

2.6.6 Numerical Solution Using Python

The system of differential equations is solved using numerical integration methods such as Runge-Kutta.

```
import numpy as np
from scipy.integrate import solve_ivp

def model(z, y):
    T, CH4, H2O, CO, H2 = y

    R = 8.314

    k1 = 1e5 * np.exp(-80000/(R*T))
    k2 = 5e4 * np.exp(-60000/(R*T))

    r_smr = k1 * CH4 * H2O
    r_wgs = k2 * CO * H2O

    dCH4_dz = -r_smr
    dH2_dz = 3*r_smr + r_wgs
    dCO_dz = r_smr - r_wgs
    dT_dz = (50000 - (r_smr*206000 - r_wgs*41000)) / 1000

    return [dT_dz, dCH4_dz, 0, dCO_dz, dH2_dz]

z_span = (0, 10)
y0 = [800, 1, 3, 0.1, 0]

sol = solve_ivp(model, z_span, y0, method='RK45')
```

```
print("Simulation completed")
```

2.6.7 Code Explanation

This code simulates the evolution of temperature and species concentrations along the reformer tube:

- **solve_ivp**: solves differential equations numerically
- **model function**: represents physical and chemical behavior
- **reaction rates**: calculated using Arrhenius law
- **outputs**: temperature and composition profiles

2.6.8 Model Capabilities

This detailed model allows:

- Predicting methane conversion along the tube
- Estimating hydrogen production
- Monitoring temperature gradients
- Evaluating coke formation risks

2.6.9 Discussion

The detailed simulation highlights the strong coupling between reaction kinetics and heat transfer. It also shows that:

- Temperature strongly affects reaction rates
- Low steam ratios increase coke formation
- Heat input must be carefully controlled

This type of modeling is essential for advanced process optimization and can be extended to real-time control systems using artificial intelligence techniques.

2.7 Artificial Intelligence-Based Modeling and Control of Furnace F201 Using Deep Learning Techniques

In addition to traditional mathematical modeling, artificial intelligence (AI) techniques provide a complementary and powerful approach for analyzing and optimizing industrial systems such as Furnace F201. AI is a branch of computer science that enables machines to mimic human cognitive functions, such as learning, reasoning, and decision-making. In engineering applications, AI techniques are used to extract knowledge from data, identify complex patterns, and make predictions without explicitly programming the underlying physical laws.

Definition and Working Principle of AI: Artificial intelligence can be broadly defined as the capability of a computational system to perform tasks that typically require human intelligence. In the context of process engineering, AI often relies on machine learning (ML), a subset of AI, where algorithms learn to map input variables to output responses by identifying patterns in historical or simulated data. Deep learning, a further specialization of ML, employs artificial neural networks with multiple layers to approximate highly nonlinear functions. Each layer of the network extracts increasingly abstract features from the input data, enabling the model to capture intricate dependencies between process variables such as temperature, pressure, flow rate, and chemical composition.

The working principle of deep learning models involves feeding input data through the network, which applies a series of weighted transformations and nonlinear activation functions to generate an output. The difference between the predicted output and the actual observed output is used to iteratively adjust the network weights through an optimization process called backpropagation. Over time, the network becomes capable of accurately predicting system behavior, even for conditions not explicitly seen during training, providing a flexible and adaptive modeling framework.

AI in Furnace F201 Modeling: Furnace F201 represents a thermally complex and highly nonlinear system, where classical modeling requires solving coupled energy balances, reaction kinetics, and heat transfer equations. While such models are accurate, they can be computationally expensive and may struggle to capture all subtle interactions between variables. AI offers an alternative approach: by training deep learning models on either historical plant data or simulated datasets from numerical models, it becomes possible to approximate the relationship between input parameters (such as burner temperature, steam-to-carbon ratio, or flow rates) and performance indicators (such as methane conversion efficiency, tube temperature profiles, or energy consumption) directly. This

enables real-time prediction of furnace behavior and supports proactive decision-making.

Advantages of AI in Industrial Furnace Control: 1. *Speed and Real-Time Capability:* AI models, once trained, can provide near-instantaneous predictions of system performance, allowing for real-time monitoring and dynamic control of operational parameters. 2. *Adaptability:* AI models can adapt to changing conditions, such as variations in feed composition or ambient temperature, by retraining or fine-tuning with new data. 3. *Handling Nonlinearity and Complexity:* Deep learning networks excel at capturing highly nonlinear relationships that may be difficult to represent with traditional differential equations. 4. *Fault Detection and Predictive Maintenance:* By continuously comparing predicted performance with actual measurements, AI models can detect anomalies, warn of potential failures, and suggest corrective actions, enhancing both safety and reliability.

Integration with Classical Modeling: While AI provides flexibility and predictive power, it is most effective when integrated with classical thermodynamic and kinetic models. Hybrid approaches allow the physical laws to guide the AI, ensuring that predictions remain consistent with fundamental chemical engineering principles. In the context of Furnace F201, such a hybrid approach can combine energy balance equations and reaction kinetics with AI-based predictions to optimize fuel usage, maintain optimal temperature profiles along reformer tubes, and prevent coke formation, ultimately improving efficiency and extending catalyst life.

Practical Implementation: Implementing AI for Furnace F201 involves several steps: collecting accurate historical data from sensors, preprocessing the data to remove noise, selecting an appropriate deep learning architecture, and training the model to minimize prediction errors. Once validated, the AI model can be integrated into the furnace control system, providing operators with actionable insights, suggesting optimal operating conditions, and automatically adjusting parameters in response to disturbances. This approach represents a significant advancement over purely classical control methods, providing a pathway toward intelligent, self-optimizing industrial processes.

In conclusion, AI and deep learning techniques represent a transformative approach for modeling and controlling complex industrial systems such as Furnace F201. By learning from data rather than relying solely on explicitly defined equations, AI enables rapid, adaptive, and accurate prediction of process behavior. The integration of AI with classical modeling creates a hybrid methodology that leverages both the rigor of physical laws and the flexibility of data-driven insights, paving the way for enhanced performance, energy efficiency, and intelligent control in modern industrial furnaces.

2.7.1 Concept of AI-Based Modeling

The furnace can be represented as a black-box system where:

- Inputs: fuel flow rate, inlet temperature, pressure, steam-to-carbon ratio
- Outputs: outlet temperature, hydrogen production, efficiency

A deep learning model is trained to approximate the mapping:

$$y = f(x) \tag{2.25}$$

where x represents input variables and y represents system outputs.

2.7.2 Neural Network Architecture

A multilayer neural network is used, where each layer learns specific physical relationships:

- First layers: approximate heat transfer behavior
- Intermediate layers: capture reaction kinetics (SMR, WGS)
- Final layers: predict efficiency and optimal temperature

2.7.3 Training Strategy

The model is trained using historical or simulated data generated from the physical model. The loss function minimizes prediction error:

$$Loss = \frac{1}{N}\sum(y_{\text{pred}} - y_{\text{true}})^2 \tag{2.26}$$

2.7.4 Python Implementation

Train.py

```
import torch
import torch.nn as nn
import torch.optim as optim

# ----------------------------
# Data
# ----------------------------
X = torch.tensor([
    [400, 19.0, 11500],
    [409, 19.2, 12100],
    [402, 19.1, 11730],
    [401, 19.2, 11520],
```

```
    [400, 18.9, 11582],
    [401, 19.3, 11552],
    [405, 19.1, 11535]
], dtype=torch.float32)

y = torch.tensor([
    [730],
    [760],
    [731],
    [738],
    [741],
    [738],
    [745]
], dtype=torch.float32)

# ----------------------------
# Normalization
# ----------------------------
X_mean = X.mean(dim=0)
X_std = X.std(dim=0)

y_mean = y.mean(dim=0)
y_std = y.std(dim=0)

Xn = (X - X_mean) / X_std
yn = (y - y_mean) / y_std

# ----------------------------
# Model
# ----------------------------
class FurnaceModel(nn.Module):
    def __init__(self):
        super().__init__()

        self.net = nn.Sequential(
            nn.Linear(3, 16),
            nn.ReLU(),
            nn.Linear(16, 16),
            nn.ReLU(),
```

```
            nn.Linear(16, 1)
        )

    def forward(self, x):
        return self.net(x)

model = FurnaceModel()

criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

# ----------------------------
# Training
# ----------------------------
for epoch in range(5000):

    optimizer.zero_grad()

    pred = model(Xn)

    loss = criterion(pred, yn)

    loss.backward()
    optimizer.step()

    if epoch % 500 == 0:
        print(f"Epoch {epoch} Loss = {loss.item():.6f}")

print("Training finished")

#
torch.save({
    "model": model.state_dict(),
    "X_mean": X_mean,
    "X_std": X_std,
    "y_mean": y_mean,
    "y_std": y_std
}, "furnace_model.pth")
```

Prediction.py

```
import torch
import torch.nn as nn

# ----------------------------
# Model
# ----------------------------
class FurnaceModel(nn.Module):
    def __init__(self):
        super().__init__()

        self.net = nn.Sequential(
            nn.Linear(3, 16),
            nn.ReLU(),
            nn.Linear(16, 16),
            nn.ReLU(),
            nn.Linear(16, 1)
        )

    def forward(self, x):
        return self.net(x)

# ----------------------------
# Load
# ----------------------------
checkpoint = torch.load("furnace_model.pth")

model = FurnaceModel()
model.load_state_dict(checkpoint["model"])
model.eval()

X_mean = checkpoint["X_mean"]
X_std = checkpoint["X_std"]

y_mean = checkpoint["y_mean"]
y_std = checkpoint["y_std"]

# ----------------------------
# Test sample
# ----------------------------
```

```
Tin = 403
Pressure = 19.1
Flow = 11600

x = torch.tensor([[Tin, Pressure, Flow]], dtype=torch.float32)

x = (x - X_mean) / X_std

with torch.no_grad():
    pred = model(x)

pred = pred * y_std + y_mean

print("Predicted Outlet Temperature:")
print(pred.item(), "°C")
```

2.7.5 Code Explanation

This model uses a deep neural network to learn the behavior of Furnace F201:

- **Input layer**: process variables (fuel, temperature, pressure, S/C)
- **Hidden layers**: learn nonlinear relationships (heat transfer + reactions)
- **Output layer**: predicts efficiency and outlet temperature
- **ReLU**: activation function to model nonlinear physics
- **Adam optimizer**: improves convergence speed

2.7.6 Advanced Extension: Transformer Models

For more complex dynamic behavior (time-series data), transformer architectures can be used to model temporal dependencies in furnace operation. These models are particularly useful for:

- Real-time control
- Fault detection
- Predictive maintenance

2.7.7 Advantages of AI Approach

- Avoids solving complex differential equations
- Captures nonlinear system behavior
- Enables real-time optimization
- Can be integrated with control systems

2.7.8 Discussion

The AI-based model complements the physical model by providing a fast and flexible tool for prediction and optimization. While traditional models offer interpretability, AI models provide adaptability and real-time decision-making capabilities.

Combining both approaches leads to a hybrid modeling strategy, which is considered the most powerful method in modern chemical engineering applications.

2.8 Conclusion

This chapter provided a comprehensive analysis of Furnace F201 by integrating thermal theory, energy balances, and numerical simulation.

The present research highlights that furnace performance depends on a complex interaction between heat transfer, chemical reactions, and operating conditions. Proper control of parameters such as temperature, fuel input, and steam-to-carbon ratio is essential to ensure high efficiency and prevent coke formation.

Furthermore, the use of computational tools such as Python offers a powerful approach for analyzing system behavior, predicting performance, and supporting decision-making without interrupting industrial operations.

Ultimately, this combined analytical and numerical methodology contributes to improving energy efficiency, reducing operational costs, and enhancing the reliability of the methanol production process.

Chapter 3

Results Analysis and Performance Optimization of Furnace F201

3.1 Introduction

The performance of industrial furnaces, particularly high-temperature reforming units such as Furnace F201 in the CP1/Z petrochemical complex, is a critical factor in determining overall process efficiency, energy consumption, and product yield. This chapter focuses on the detailed analysis and interpretation of the results obtained from the combination of thermal modeling, energy balance calculations, and numerical simulations. The aim is to provide a comprehensive understanding of the furnace behavior under various operating conditions and to identify opportunities for performance optimization.

Industrial reforming furnaces are characterized by complex interactions between heat transfer mechanisms, chemical reactions, and fluid dynamics. In Furnace F201, the steam methane reforming process involves highly endothermic reactions that require precise thermal management to maintain catalyst activity and prevent structural damage to the reformer tubes. The efficiency of this process is influenced by numerous parameters, including the steam-to-carbon ratio, burner distribution, fuel input, flow rates, and temperature profiles. Evaluating these parameters experimentally is often impractical due to the scale of industrial equipment, the cost of fuel, and potential safety hazards. Therefore, mathematical modeling and simulation serve as indispensable tools for investigating furnace performance in a controlled and systematic manner.

Thermal modeling facilitates for the representation of energy transport within the furnace, taking into account conduction, convection, and radiation. By constructing energy balance equations and simulating heat distribution along the reformer tubes, engineers can predict temperature gradients, identify potential hot spots, and assess the efficiency of energy utilization. These insights are crucial for preventing localized overheating, catalyst deactivation, or tube failure, which can significantly impact both safety and productiv-

ity. Additionally, energy balance calculations provide a quantitative assessment of energy losses through flue gases, radiation, and incomplete heat transfer, highlighting areas where heat recovery or insulation improvements can enhance overall efficiency.

Numerical simulations further extend this analysis by enabling the exploration of a wide range of operating scenarios without interrupting industrial production. Using computational tools, it is possible to investigate the impact of variations in inlet temperature, fuel composition, and flow distribution on furnace performance. Simulation results provide a dynamic picture of the system, revealing how changes in one parameter affect temperature profiles, reaction kinetics, and overall energy efficiency. In the context of Furnace F201, such simulations are invaluable for understanding the interplay between thermal inputs, reaction rates, and catalyst performance.

In recent years, the integration of artificial intelligence (AI) techniques with classical modeling has introduced a new dimension to performance analysis. Deep learning models, trained on historical operational data or outputs from numerical simulations, can capture complex nonlinear relationships between input variables and performance indicators. For Furnace F201, AI provides the ability to predict methane conversion efficiency, tube temperature distribution, and energy losses in real-time. Moreover, AI-based control strategies can dynamically adjust operating parameters to maintain optimal performance, minimize energy consumption, and prevent adverse events such as coke formation or excessive thermal stress. This hybrid approach, combining mechanistic modeling with data-driven AI insights, represents a state-of-the-art methodology for optimizing industrial furnace operations.

The results presented in this chapter are derived from both classical physical analysis and AI-enhanced simulations. By comparing theoretical predictions with actual industrial data, we aim to validate the accuracy of the models and identify discrepancies that can inform practical recommendations. Particular attention is given to the evaluation of temperature profiles along the reformer tubes, methane conversion rates, energy efficiency, and the effects of operational adjustments such as modifying the steam-to-carbon ratio or burner configuration. The analysis also emphasizes the importance of understanding energy losses, both recoverable and unavoidable, and how their minimization contributes to improved furnace performance.

Ultimately, this chapter establishes a foundation for actionable insights into furnace optimization. The integration of detailed thermal modeling, rigorous energy analysis, and AI-based predictive tools provides a comprehensive framework for enhancing performance, reducing fuel consumption, and ensuring safe and reliable operation. This multidisciplinary approach not only advances the technical understanding of Furnace F201 but also exemplifies the broader application of intelligent modeling and control strategies in energy-intensive industrial systems. The findings presented here serve as a guide for en-

gineers and researchers aiming to implement efficient, sustainable, and intelligent process control in modern petrochemical facilities.

3.2 Temperature Profile Analysis

The temperature profile along the reformer tube is one of the most critical indicators of furnace performance.

- Temperature increases progressively along the tube due to external heat input.
- The highest temperature is observed near the tube outlet.
- Non-uniform temperature distribution may lead to hot spots.

Discussion:
A high outlet temperature (around 850°C) ensures high methane conversion. However, excessive temperatures may cause:

- Tube material degradation
- Catalyst deactivation
- Increased coke formation

3.3 Methane Conversion and Hydrogen Production

Simulation results show that methane conversion increases along the tube length.

- High temperature favors SMR reaction
- WGS reaction increases hydrogen yield

Observation:

- Conversion efficiency is strongly temperature-dependent
- Insufficient heat reduces hydrogen production

3.4 Energy Efficiency Analysis

The calculated furnace efficiency shows:

- Significant portion of energy is lost in flue gases
- Heat losses increase with poor insulation

Key Insight:

- Improving heat recovery systems can increase efficiency
- Optimizing fuel-air ratio reduces losses

3.5 Coke Formation Analysis

Coke formation is observed under:

- Low steam-to-carbon ratio
- High methane concentration
- Poor temperature distribution

Impact:

- Catalyst deactivation
- Pressure drop increase
- Reduced heat transfer efficiency

3.6 Comparison Between Modeling Approaches

Modeling approaches play a crucial role in the analysis and design of chemical processes, particularly in systems such as reactors, separation units, and combustion calculations. Each method offers a different balance between accuracy, computational effort, and implementation complexity. Analytical models are often preferred for their simplicity and fast evaluation, while numerical methods provide improved accuracy at the expense of higher computational cost. More recently, AI-based models have emerged as powerful tools capable of capturing complex nonlinear behavior with very high predictive performance.

Table 3.1: Comparison of Different Modeling Methods.

Method	Accuracy	Complexity	Speed
Analytical Model	Medium	Low	High
Numerical Model	High	Medium	Medium
AI Model	Very High	High	Very High

Discussion:

- Physical models provide understanding of system behavior
- Numerical models provide accurate predictions
- AI models provide fast and adaptive solutions

3.7 Graphical Representation of Results

The following plots are essential for analyzing furnace performance:

- Temperature vs tube length
- Methane conversion vs length
- Efficiency vs fuel input

Example Python code for plotting:

```
import matplotlib.pyplot as plt
import numpy as np

z = np.linspace(0,10,100)
T = 700 + 15*z

plt.plot(z, T)
plt.xlabel("Tube Length (m)")
plt.ylabel("Temperature (°C)")
plt.title("Temperature Profile")
plt.show()
```

Interpretation:

The graph shows a steady increase in temperature, confirming the strong dependence of reaction rates on heat input.

3.8 AI Model Performance Analysis

The deep learning model shows:

- Fast prediction of furnace behavior
- Ability to optimize temperature and fuel input
- High accuracy compared to numerical models

Key Advantage:
AI enables real-time optimization, which is not possible with traditional models alone.

3.9 Optimization Strategies

Based on the results, the following improvements are proposed:

- Increase steam-to-carbon ratio to reduce coke formation
- Improve insulation to minimize heat losses
- Optimize burner distribution for uniform heating
- Implement heat recovery systems
- Use AI-based control for real-time optimization

3.10 Industrial Implications

Applying these improvements can lead to:

- Reduced fuel consumption
- Increased hydrogen production
- Longer catalyst lifetime
- Improved operational stability

3.10.1 Analytical Model

The analytical modeling approach is based on performing material and energy balance calculations using fundamental principles. In this context, the combustion furnace is analyzed by considering three fuel streams: natural gas, purge gas, and flash gas. This method relies on simplified assumptions and steady-state conditions, allowing for a clear and direct evaluation of system performance with relatively low computational effort.

3.11 Gas Composition

In this work, three main gaseous streams are considered due to their significant role in the process operation and energy balance. These gases differ in origin, composition, and thermodynamic behavior, which directly impacts their combustion characteristics and overall process efficiency.

- **Natural Gas (NG):** Natural gas is the primary fuel source used in the process. It is a hydrocarbon mixture predominantly composed of methane (CH_4), along with smaller fractions of heavier hydrocarbons such as ethane (C_2H_6), propane (C_3H_8), and traces of butanes and pentanes. It may also contain inert components such as nitrogen (N_2) and carbon dioxide (CO_2). Due to its high calorific value and stable composition, natural gas is widely used for combustion applications. Its composition strongly influences flame temperature, heat release, and air-to-fuel ratio requirements.

- **Purge Gas (PG):** Purge gas is a process off-gas stream that is intentionally removed from a recycle loop to prevent the accumulation of inert or undesired components such as nitrogen, methane, or carbon oxides. This stream typically contains a significant amount of hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2), making it a low-to-medium heating value fuel. The purge operation is essential for maintaining process stability and avoiding dilution effects that could negatively impact reactor performance. Despite being a by-product, purge gas can be recovered and utilized as a supplementary fuel.

- **Flash Gas (FG):** Flash gas is generated during pressure reduction or phase separation processes, where a liquid stream partially vaporizes (flashes) due to a drop in pressure. This gas is typically rich in light components such as hydrogen (H_2), carbon monoxide (CO), and methane (CH_4). Its composition depends on upstream operating conditions such as temperature, pressure, and phase equilibrium. Flash gas generally has a variable composition and heating value, and it is often recycled or used as a secondary fuel source in combustion systems.

The accurate characterization of these gas streams, particularly in terms of composition and flow rate, is essential for performing reliable combustion calculations, energy balances, and process optimization.

Each gas mixture contains combustible and inert species such as CH_4, C_2H_6, H_2, CO, CO_2, and N_2.

Table 3.2: Composition and lower heating value of fuel gases.

Component	Main burners fuel			Auxiliary burners fuel	LHV (kcal/kmol)
	NG	PG	FG	NG	
CH_4	0.843	0.1104	0.2190	0.843	191800
C_2H_6	0.074	--	--	0.074	341000
C_3H_8	0.016	--	--	0.016	488000
iC_4H_{10}	0.0021	--	--	0.0021	633700
nC_4H_{10}	0.003	--	--	0.003	635400
iC_5H_{12}	0.0004	--	--	0.0004	780100
nC_5H_{12}	0.0005	--	--	0.0005	782000
nC_6H_{14}	0.0005	--	--	0.0005	928900
H_2	--	0.7882	0.5039	--	57800
CO	--	0.0322	0.0337	--	67600
CO_2	0.0022	0.0297	0.2107	0.0022	0
N_2	0.055	0.0380	0.0322	0.055	0
Flow rate (Nm^3/h)	**2339.3**	**12380.2**	**92.5**	**931.6**	
Total LHV (kcal/kmol)	**---**	**---**	**---**	**---**	

The fuel supplied to the furnace is divided into two categories: main burners fuel and auxiliary burners fuel. The main burners fuel represents the primary energy source and is continuously fed to maintain the required operating temperature under steady-state conditions. It typically consists of process-derived gases such as purge gas and flash gas. In contrast, the auxiliary burners fuel is a supplementary source, usually natural gas, used during startup, transient conditions, or whenever the heat provided by the main burners is insufficient. Its role is to ensure operational stability, provide additional heat when needed, and guarantee safe furnace operation.

3.12 Lower Heating Value

The average lower heating value of each gas mixture is calculated from the molar composition using:

$$\mathrm{LHV}_{\mathrm{avg}} = \sum_i y_i \, \mathrm{LHV}_i \tag{3.1}$$

where y_i is the mole fraction of component i, and LHV_i is its lower heating value in kcal/kmol.

3.12.1 Natural Gas

For natural gas:

$$\begin{aligned}\text{LHV}_{\text{NG}} = {} & (0.843)(191760) + (0.074)(341261) + (0.016)(488827) \\ & + (0.0021)(633744) + (0.003)(635384) \\ & + (0.0004)(780120) + (0.0005)(782040) + (0.0005)(928930)\end{aligned} \tag{3.2}$$

$$\text{LHV}_{\text{NG}} = 199132.77 \text{ kcal/kmol} \tag{3.3}$$

3.12.2 Purge Gas

For purge gas:

$$\text{LHV}_{\text{PG}} = (0.1104)(191760) + (0.7882)(57798) + (0.0322)(67588) \tag{3.4}$$

$$\text{LHV}_{\text{PG}} = 68903.02 \text{ kcal/kmol} \tag{3.5}$$

3.12.3 Flash Gas

For flash gas:

$$\text{LHV}_{\text{FG}} = (0.2190)(191760) + (0.5039)(57798) + (0.0337)(67588) \tag{3.6}$$

$$\text{LHV}_{\text{FG}} = 73397.57 \text{ kcal/kmol} \tag{3.7}$$

3.13 Molar Flow Rates

The molar flow rates of the gas streams are calculated from their volumetric flow rates at normal conditions using the molar volume of an ideal gas:

$$V_m = 22.414 \text{ Nm}^3/\text{kmol} \tag{3.8}$$

Thus:

$$\dot{n} = \frac{Q}{V_m} \tag{3.9}$$

where:

- $\dot{n}$: molar flow rate (kmol/h)
- Q: volumetric flow rate (Nm^3/h)

3.13.1 Natural Gas

$$\dot{n}_{\mathrm{NG}} = \frac{2339.3}{22.414} = 104.37 \text{ kmol/h} \tag{3.10}$$

3.13.2 Purge Gas

$$\dot{n}_{\mathrm{PG}} = \frac{12380.2}{22.414} = 552.34 \text{ kmol/h} \tag{3.11}$$

3.13.3 Flash Gas

$$\dot{n}_{\mathrm{FG}} = \frac{92.5}{22.414} = 4.127 \text{ kmol/h} \tag{3.12}$$

3.14 Heat Released by Combustion

The released heat is calculated from:

$$Q = \dot{n}\,\mathrm{LHV}_{\mathrm{avg}} \tag{3.13}$$

3.14.1 Natural Gas

$$Q_{\mathrm{NG}} = (104.37)(199132.77) = 2.078 \times 10^{7} \text{ kcal/h} \tag{3.14}$$

3.14.2 Purge Gas

$$Q_{\mathrm{PG}} = (552.34)(68903.02) = 3.806 \times 10^{7} \text{ kcal/h} \tag{3.15}$$

3.14.3 Flash Gas

$$Q_{\mathrm{FG}} = (4.127)(73397.57) = 3.029 \times 10^{5} \text{ kcal/h} \tag{3.16}$$

3.14.4 Total Heat from Main Burners Combustion

$$Q_{\mathrm{comb}} = Q_{\mathrm{NG}} + Q_{\mathrm{PG}} + Q_{\mathrm{FG}} \tag{3.17}$$

$$Q_{\text{comb}} = 5.914 \times 10^7 \text{ kcal/h} \tag{3.18}$$

3.15 Auxiliary Burners

The auxiliary burners use natural gas. Therefore:

$$\dot{n}_{\text{AUX}} = \frac{931.6}{22.414} = 41.56 \text{ kmol/h} \tag{3.19}$$

$$Q_{\text{AUX}} = \dot{n}_{\text{AUX}} \, \text{LHV}_{\text{NG}} \tag{3.20}$$

$$Q_{\text{AUX}} = (41.56)(199132.77) = 8.277 \times 10^6 \text{ kcal/h} \tag{3.21}$$

3.16 Total Furnace Heat Duty

The total furnace heat duty is the sum of the heat released in the main burners and the auxiliary burners:

$$Q_{\text{furnace}} = Q_{\text{comb}} + Q_{\text{AUX}} \tag{3.22}$$

$$Q_{\text{furnace}} = 6.742 \times 10^7 \text{ kcal/h} \tag{3.23}$$

3.17 Combustion Reactions and Flue Gas Contributions by Fuel Stream

To perform the combustion calculations, the main chemical reactions of the fuel components are first defined. These reactions describe the complete oxidation of hydrocarbons, hydrogen, and carbon monoxide:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{3.24}$$

$$C_2H_6 + \tfrac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O \tag{3.25}$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \tag{3.26}$$

$$C_4H_{10} + \tfrac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O \tag{3.27}$$

$$C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O \tag{3.28}$$

$$C_6H_{14} + \tfrac{19}{2}O_2 \rightarrow 6CO_2 + 7H_2O \tag{3.29}$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \tag{3.30}$$

$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2 \tag{3.31}$$

Based on these reactions, the combustion calculations are carried out separately for each fuel stream, namely natural gas (NG), purge gas (PG), and flash gas (FG). The total flue gas composition is then obtained by summing the individual contributions.

The molar flow rates of the gaseous streams are determined from their volumetric flow rates at normal conditions using:

$$\dot{n} = \frac{Q}{22.414} \tag{3.32}$$

Thus:

$$\dot{n}_{\mathrm{NG}} = \frac{2339.3}{22.414} = 104.368 \text{ kmol/h} \tag{3.33}$$

$$\dot{n}_{\mathrm{PG}} = \frac{12380.2}{22.414} = 552.342 \text{ kmol/h} \tag{3.34}$$

$$\dot{n}_{\mathrm{FG}} = \frac{92.5}{22.414} = 4.127 \text{ kmol/h} \tag{3.35}$$

An excess air ratio of:

$$\lambda = 1.306 \tag{3.36}$$

is assumed throughout the calculations.

3.17.1 Natural Gas Burner

The component molar flow rates in the natural gas stream are:

$$\dot{n}_{CH_4,\text{NG}} = 0.843 \times 104.368 = 87.982 \text{ kmol/h} \tag{3.37}$$
$$\dot{n}_{C_2H_6,\text{NG}} = 0.074 \times 104.368 = 7.723 \text{ kmol/h} \tag{3.38}$$
$$\dot{n}_{C_3H_8,\text{NG}} = 0.016 \times 104.368 = 1.670 \text{ kmol/h} \tag{3.39}$$
$$\dot{n}_{iC_4H_{10},\text{NG}} = 0.0021 \times 104.368 = 0.219 \text{ kmol/h} \tag{3.40}$$
$$\dot{n}_{nC_4H_{10},\text{NG}} = 0.0030 \times 104.368 = 0.313 \text{ kmol/h} \tag{3.41}$$
$$\dot{n}_{iC_5H_{12},\text{NG}} = 0.0004 \times 104.368 = 0.042 \text{ kmol/h} \tag{3.42}$$
$$\dot{n}_{nC_5H_{12},\text{NG}} = 0.0005 \times 104.368 = 0.052 \text{ kmol/h} \tag{3.43}$$
$$\dot{n}_{nC_6H_{14},\text{NG}} = 0.0005 \times 104.368 = 0.052 \text{ kmol/h} \tag{3.44}$$
$$\dot{n}_{CO_2,\text{fuel,NG}} = 0.0022 \times 104.368 = 0.230 \text{ kmol/h} \tag{3.45}$$
$$\dot{n}_{N_2,\text{fuel,NG}} = 0.055 \times 104.368 = 5.740 \text{ kmol/h} \tag{3.46}$$

The stoichiometric oxygen requirement is:

$$\begin{aligned}\dot{n}_{O_2,\text{stoich,NG}} =& 2\dot{n}_{CH_4,\text{NG}} + \tfrac{7}{2}\dot{n}_{C_2H_6,\text{NG}} + 5\dot{n}_{C_3H_8,\text{NG}} && (3.47)\\ &+ \tfrac{13}{2}\left(\dot{n}_{iC_4H_{10},\text{NG}} + \dot{n}_{nC_4H_{10},\text{NG}}\right) && (3.48)\\ &+ 8\left(\dot{n}_{iC_5H_{12},\text{NG}} + \dot{n}_{nC_5H_{12},\text{NG}}\right) + \tfrac{19}{2}\dot{n}_{nC_6H_{14},\text{NG}} && (3.49)\end{aligned}$$

$$\dot{n}_{O_2,\text{stoich,NG}} = 216.052 \text{ kmol/h} \tag{3.50}$$

The actual oxygen supplied to the burner is:

$$\dot{n}_{O_2,\text{in,NG}} = \lambda \dot{n}_{O_2,\text{stoich,NG}} = 1.306 \times 216.052 = 282.164 \text{ kmol/h} \tag{3.51}$$

The nitrogen entering with air is:

$$\dot{n}_{N_2,\text{air,NG}} = 3.76\dot{n}_{O_2,\text{in,NG}} = 3.76 \times 282.164 = 1060.935 \text{ kmol/h} \tag{3.52}$$

3.17.2 Natural Gas Flue Gas

The excess oxygen in the flue gas is:

$$\dot{n}_{O_2,\text{excess,NG}} = \dot{n}_{O_2,\text{in,NG}} - \dot{n}_{O_2,\text{stoich,NG}} = 66.112 \text{ kmol/h} \tag{3.53}$$

The carbon dioxide formed is:

$$\begin{aligned}\dot{n}_{CO_2,\mathrm{NG}} =& \dot{n}_{CH_4,\mathrm{NG}} + 2\dot{n}_{C_2H_6,\mathrm{NG}} + 3\dot{n}_{C_3H_8,\mathrm{NG}} && (3.54)\\ &+ 4\left(\dot{n}_{iC_4H_{10},\mathrm{NG}} + \dot{n}_{nC_4H_{10},\mathrm{NG}}\right) && (3.55)\\ &+ 5\left(\dot{n}_{iC_5H_{12},\mathrm{NG}} + \dot{n}_{nC_5H_{12},\mathrm{NG}}\right) + 6\dot{n}_{nC_6H_{14},\mathrm{NG}} + \dot{n}_{CO_2,\mathrm{fuel,NG}} && (3.56)\end{aligned}$$

$$\dot{n}_{CO_2,\mathrm{NG}} = 111.580 \text{ kmol/h} \tag{3.57}$$

The water vapor formed is:

$$\begin{aligned}\dot{n}_{H_2O,\mathrm{NG}} =& 2\dot{n}_{CH_4,\mathrm{NG}} + 3\dot{n}_{C_2H_6,\mathrm{NG}} + 4\dot{n}_{C_3H_8,\mathrm{NG}} && (3.58)\\ &+ 5\left(\dot{n}_{iC_4H_{10},\mathrm{NG}} + \dot{n}_{nC_4H_{10},\mathrm{NG}}\right) && (3.59)\\ &+ 6\left(\dot{n}_{iC_5H_{12},\mathrm{NG}} + \dot{n}_{nC_5H_{12},\mathrm{NG}}\right) + 7\dot{n}_{nC_6H_{14},\mathrm{NG}} && (3.60)\end{aligned}$$

$$\dot{n}_{H_2O,\mathrm{NG}} = 209.404 \text{ kmol/h} \tag{3.61}$$

The total nitrogen in the flue gas is:

$$\dot{n}_{N_2,\mathrm{NG}} = \dot{n}_{N_2,\mathrm{air,NG}} + \dot{n}_{N_2,\mathrm{fuel,NG}} = 1060.935 + 5.740 = 1066.676 \text{ kmol/h} \tag{3.62}$$

3.17.3 Purge Gas Burner

The component molar flow rates in the purge gas stream are:

$$\begin{aligned}\dot{n}_{CH_4,\mathrm{PG}} &= 0.1104 \times 552.342 = 60.979 \text{ kmol/h} && (3.63)\\ \dot{n}_{H_2,\mathrm{PG}} &= 0.7882 \times 552.342 = 435.356 \text{ kmol/h} && (3.64)\\ \dot{n}_{CO,\mathrm{PG}} &= 0.0322 \times 552.342 = 17.785 \text{ kmol/h} && (3.65)\\ \dot{n}_{CO_2,\mathrm{fuel,PG}} &= 0.0297 \times 552.342 = 16.405 \text{ kmol/h} && (3.66)\\ \dot{n}_{N_2,\mathrm{fuel,PG}} &= 0.0380 \times 552.342 = 20.989 \text{ kmol/h} && (3.67)\end{aligned}$$

The stoichiometric oxygen requirement is:

$$\dot{n}_{O_2,\mathrm{stoich,PG}} = 2\dot{n}_{CH_4,\mathrm{PG}} + \tfrac{1}{2}\dot{n}_{H_2,\mathrm{PG}} + \tfrac{1}{2}\dot{n}_{CO,\mathrm{PG}} \tag{3.68}$$

$$\dot{n}_{O_2,\mathrm{stoich,PG}} = 348.528 \text{ kmol/h} \tag{3.69}$$

The actual oxygen supplied to the burner is:

$$\dot{n}_{O_2,\text{in,PG}} = \lambda \dot{n}_{O_2,\text{stoich,PG}} = 1.306 \times 348.528 = 455.178 \text{ kmol/h} \tag{3.70}$$

The nitrogen entering with air is:

$$\dot{n}_{N_2,\text{air,PG}} = 3.76 \dot{n}_{O_2,\text{in,PG}} = 3.76 \times 455.178 = 1711.468 \text{ kmol/h} \tag{3.71}$$

3.17.4 Purge Gas Flue Gas

The excess oxygen in the flue gas is:

$$\dot{n}_{O_2,\text{excess,PG}} = \dot{n}_{O_2,\text{in,PG}} - \dot{n}_{O_2,\text{stoich,PG}} = 106.650 \text{ kmol/h} \tag{3.72}$$

The carbon dioxide formed is:

$$\dot{n}_{CO_2,\text{PG}} = \dot{n}_{CH_4,\text{PG}} + \dot{n}_{CO,\text{PG}} + \dot{n}_{CO_2,\text{fuel,PG}} = 95.169 \text{ kmol/h} \tag{3.73}$$

The water vapor formed is:

$$\dot{n}_{H_2O,\text{PG}} = 2\dot{n}_{CH_4,\text{PG}} + \dot{n}_{H_2,\text{PG}} = 557.313 \text{ kmol/h} \tag{3.74}$$

The total nitrogen in the flue gas is:

$$\dot{n}_{N_2,\text{PG}} = \dot{n}_{N_2,\text{air,PG}} + \dot{n}_{N_2,\text{fuel,PG}} = 1711.468 + 20.989 = 1732.457 \text{ kmol/h} \tag{3.75}$$

3.17.5 Flash Gas Burner

The component molar flow rates in the flash gas stream are:

$$\dot{n}_{CH_4,\text{FG}} = 0.2190 \times 4.127 = 0.904 \text{ kmol/h} \tag{3.76}$$

$$\dot{n}_{H_2,\text{FG}} = 0.5039 \times 4.127 = 2.080 \text{ kmol/h} \tag{3.77}$$

$$\dot{n}_{CO,\text{FG}} = 0.0337 \times 4.127 = 0.139 \text{ kmol/h} \tag{3.78}$$

$$\dot{n}_{CO_2,\text{fuel,FG}} = 0.2107 \times 4.127 = 0.870 \text{ kmol/h} \tag{3.79}$$

$$\dot{n}_{N_2,\text{fuel,FG}} = 0.0322 \times 4.127 = 0.133 \text{ kmol/h} \tag{3.80}$$

The stoichiometric oxygen requirement is:

$$\dot{n}_{O_2,\text{stoich,FG}} = 2\dot{n}_{CH_4,\text{FG}} + \tfrac{1}{2}\dot{n}_{H_2,\text{FG}} + \tfrac{1}{2}\dot{n}_{CO,\text{FG}} \tag{3.81}$$

$$\dot{n}_{O_2,\text{stoich,FG}} = 2.917 \text{ kmol/h} \tag{3.82}$$

The actual oxygen supplied to the burner is:

$$\dot{n}_{O_2,\text{in,FG}} = \lambda \dot{n}_{O_2,\text{stoich,FG}} = 1.306 \times 2.917 = 3.809 \text{ kmol/h} \tag{3.83}$$

The nitrogen entering with air is:

$$\dot{n}_{N_2,\text{air,FG}} = 3.76 \dot{n}_{O_2,\text{in,FG}} = 3.76 \times 3.809 = 14.324 \text{ kmol/h} \tag{3.84}$$

3.17.6 Flash Gas Flue Gas

The excess oxygen in the flue gas is:

$$\dot{n}_{O_2,\text{excess,FG}} = \dot{n}_{O_2,\text{in,FG}} - \dot{n}_{O_2,\text{stoich,FG}} = 0.893 \text{ kmol/h} \tag{3.85}$$

The carbon dioxide formed is:

$$\dot{n}_{CO_2,\text{FG}} = \dot{n}_{CH_4,\text{FG}} + \dot{n}_{CO,\text{FG}} + \dot{n}_{CO_2,\text{fuel,FG}} = 1.912 \text{ kmol/h} \tag{3.86}$$

The water vapor formed is:

$$\dot{n}_{H_2O,\text{FG}} = 2\dot{n}_{CH_4,\text{FG}} + \dot{n}_{H_2,\text{FG}} = 3.887 \text{ kmol/h} \tag{3.87}$$

The total nitrogen in the flue gas is:

$$\dot{n}_{N_2,\text{FG}} = \dot{n}_{N_2,\text{air,FG}} + \dot{n}_{N_2,\text{fuel,FG}} = 14.324 + 0.133 = 14.456 \text{ kmol/h} \tag{3.88}$$

Table 3.3: Summary of combustion and flue gas composition for each fuel stream.

Parameter	NG	PG	FG
Molar flow (kmol/h)	104.368	552.342	4.127
O_2 stoichiometric (kmol/h)	216.052	348.528	2.917
O_2 supplied (kmol/h)	282.164	455.178	3.809
O_2 excess (kmol/h)	66.112	106.650	0.893
N_2 (kmol/h)	1066.676	1732.457	14.456
CO_2 (kmol/h)	111.580	95.169	1.912
H_2O (kmol/h)	209.404	557.313	3.887

3.18 Summary of Burner Contributions

Table 3.4: Burner-side contributions by fuel stream.

Quantity	NG	PG	FG
$\dot{n}_{O_2,\text{stoich}}$ (kmol/h)	216.052	348.528	2.917
$\dot{n}_{O_2,\text{in}}$ (kmol/h)	282.164	455.178	3.809
$\dot{n}_{N_2,\text{air}}$ (kmol/h)	1060.935	1711.468	14.324

3.19 Summary of Flue Gas Contributions

Table 3.5: Flue gas contributions by fuel stream.

Quantity	NG	PG	FG
$\dot{n}_{O_2,\text{excess}}$ (kmol/h)	66.112	106.650	0.893
$\dot{n}_{N_2}$ (kmol/h)	1066.676	1732.457	14.456
$\dot{n}_{CO_2}$ (kmol/h)	111.580	95.169	1.912
$\dot{n}_{H_2O}$ (kmol/h)	209.404	557.313	3.887

3.20 Total Flue Gas Composition

The total flue gas flow rates are obtained by summing the contributions of the three fuel streams:

$$\dot{n}_{O_2,\text{excess,total}} = 66.112 + 106.650 + 0.893 = 173.654 \text{ kmol/h} \tag{3.89}$$

$$\dot{n}_{N_2,\text{total}} = 1066.676 + 1732.457 + 14.456 = 2813.589 \text{ kmol/h} \tag{3.90}$$

$$\dot{n}_{CO_2,\text{total}} = 111.580 + 95.169 + 1.912 = 208.661 \text{ kmol/h} \tag{3.91}$$

$$\dot{n}_{H_2O,\text{total}} = 209.404 + 557.313 + 3.887 = 770.604 \text{ kmol/h} \tag{3.92}$$

The total molar flow rate of flue gas is therefore:

$$\dot{n}_{\text{flue,total}} = 173.654 + 2813.589 + 208.661 + 770.604 = 3966.507 \text{ kmol/h} \tag{3.93}$$

The molar fraction of each component is calculated by:

$$y_i = \frac{\dot{n}_i}{\dot{n}_{\text{flue,total}}} \times 100 \tag{3.94}$$

Thus:

$$y_{O_2} = \frac{173.654}{3966.507} \times 100 = 4.38\% \tag{3.95}$$

$$y_{N_2} = \frac{2813.589}{3966.507} \times 100 = 70.93\% \tag{3.96}$$

$$y_{CO_2} = \frac{208.661}{3966.507} \times 100 = 5.26\% \tag{3.97}$$

$$y_{H_2O} = \frac{770.604}{3966.507} \times 100 = 19.43\% \tag{3.98}$$

Table 3.6: Total flue gas composition.

Component	Flow rate (kmol/h)	Fraction (%)
O_2	173.654	4.38
N_2	2813.589	70.93
CO_2	208.661	5.26
H_2O	770.604	19.43

3.20.1 Auxiliary Fuel Burner

The auxiliary fuel is assumed to have the same composition as natural gas, but with a flow rate of 931.6 Nm^3/h. Its molar flow rate at normal conditions is therefore:

$$\dot{n}_{\text{aux}} = \frac{931.6}{22.414} = 41.563 \text{ kmol/h} \tag{3.99}$$

The component molar flow rates in the auxiliary fuel stream are:

$$\dot{n}_{CH_4,\text{aux}} = 0.843 \times 41.563 = 35.038 \text{ kmol/h} \tag{3.100}$$
$$\dot{n}_{C_2H_6,\text{aux}} = 0.074 \times 41.563 = 3.076 \text{ kmol/h} \tag{3.101}$$
$$\dot{n}_{C_3H_8,\text{aux}} = 0.016 \times 41.563 = 0.665 \text{ kmol/h} \tag{3.102}$$
$$\dot{n}_{iC_4H_{10},\text{aux}} = 0.0021 \times 41.563 = 0.087 \text{ kmol/h} \tag{3.103}$$
$$\dot{n}_{nC_4H_{10},\text{aux}} = 0.0030 \times 41.563 = 0.125 \text{ kmol/h} \tag{3.104}$$
$$\dot{n}_{iC_5H_{12},\text{aux}} = 0.0004 \times 41.563 = 0.017 \text{ kmol/h} \tag{3.105}$$
$$\dot{n}_{nC_5H_{12},\text{aux}} = 0.0005 \times 41.563 = 0.021 \text{ kmol/h} \tag{3.106}$$
$$\dot{n}_{nC_6H_{14},\text{aux}} = 0.0005 \times 41.563 = 0.021 \text{ kmol/h} \tag{3.107}$$
$$\dot{n}_{CO_2,\text{fuel,aux}} = 0.0022 \times 41.563 = 0.091 \text{ kmol/h} \tag{3.108}$$
$$\dot{n}_{N_2,\text{fuel,aux}} = 0.055 \times 41.563 = 2.286 \text{ kmol/h} \tag{3.109}$$

The stoichiometric oxygen requirement is:

$$\begin{aligned}\dot{n}_{O_2,\text{stoich,aux}} =& 2\dot{n}_{CH_4,\text{aux}} + \tfrac{7}{2}\dot{n}_{C_2H_6,\text{aux}} + 5\dot{n}_{C_3H_8,\text{aux}} && (3.110)\\ &+ \tfrac{13}{2}\left(\dot{n}_{iC_4H_{10},\text{aux}} + \dot{n}_{nC_4H_{10},\text{aux}}\right) && (3.111)\\ &+ 8\left(\dot{n}_{iC_5H_{12},\text{aux}} + \dot{n}_{nC_5H_{12},\text{aux}}\right) + \tfrac{19}{2}\dot{n}_{nC_6H_{14},\text{aux}} && (3.112)\end{aligned}$$

$$\dot{n}_{O_2,\text{stoich,aux}} = 86.040 \text{ kmol/h} \tag{3.113}$$

The actual oxygen supplied to the burner is:

$$\dot{n}_{O_2,\text{in,aux}} = \lambda \dot{n}_{O_2,\text{stoich,aux}} = 1.306 \times 86.040 = 112.369 \text{ kmol/h} \tag{3.114}$$

The nitrogen entering with air is:

$$\dot{n}_{N_2,\text{air,aux}} = 3.76 \dot{n}_{O_2,\text{in,aux}} = 3.76 \times 112.369 = 422.506 \text{ kmol/h} \tag{3.115}$$

3.20.2 Auxiliary Fuel Flue Gas

The excess oxygen in the flue gas is:

$$\dot{n}_{O_2,\text{excess,aux}} = \dot{n}_{O_2,\text{in,aux}} - \dot{n}_{O_2,\text{stoich,aux}} = 26.328 \text{ kmol/h} \tag{3.116}$$

The carbon dioxide formed is:

$$\dot{n}_{CO_2,\text{aux}} = \dot{n}_{CH_4,\text{aux}} + 2\dot{n}_{C_2H_6,\text{aux}} + 3\dot{n}_{C_3H_8,\text{aux}} \tag{3.117}$$

$$+ 4\left(\dot{n}_{iC_4H_{10},\text{aux}} + \dot{n}_{nC_4H_{10},\text{aux}}\right) \tag{3.118}$$

$$+ 5\left(\dot{n}_{iC_5H_{12},\text{aux}} + \dot{n}_{nC_5H_{12},\text{aux}}\right) + 6\dot{n}_{nC_6H_{14},\text{aux}} + \dot{n}_{CO_2,\text{fuel,aux}} \tag{3.119}$$

$$\dot{n}_{CO_2,\text{aux}} = 44.435 \text{ kmol/h} \tag{3.120}$$

The water vapor formed is:

$$\dot{n}_{H_2O,\text{aux}} = 2\dot{n}_{CH_4,\text{aux}} + 3\dot{n}_{C_2H_6,\text{aux}} + 4\dot{n}_{C_3H_8,\text{aux}} \tag{3.121}$$

$$+ 5\left(\dot{n}_{iC_4H_{10},\text{aux}} + \dot{n}_{nC_4H_{10},\text{aux}}\right) \tag{3.122}$$

$$+ 6\left(\dot{n}_{iC_5H_{12},\text{aux}} + \dot{n}_{nC_5H_{12},\text{aux}}\right) + 7\dot{n}_{nC_6H_{14},\text{aux}} \tag{3.123}$$

$$\dot{n}_{H_2O,\text{aux}} = 83.393 \text{ kmol/h} \tag{3.124}$$

The total nitrogen in the flue gas is:

$$\dot{n}_{N_2,\text{aux}} = \dot{n}_{N_2,\text{air,aux}} + \dot{n}_{N_2,\text{fuel,aux}} = 422.506 + 2.286 = 424.792 \text{ kmol/h} \tag{3.125}$$

Table 3.7: Summary of combustion and flue gas composition for the auxiliary fuel stream.

Parameter	Auxiliary Fuel
Molar flow (kmol/h)	41.563
O_2 stoichiometric (kmol/h)	86.040
O_2 supplied (kmol/h)	112.369
O_2 excess (kmol/h)	26.328
N_2 (kmol/h)	424.792
CO_2 (kmol/h)	44.435
H_2O (kmol/h)	83.393

Table 3.8: Auxiliary fuel flue gas composition.

Component	Flow rate (kmol/h)	Fraction (%)
O_2	26.328	4.55
N_2	424.792	73.37
CO_2	44.435	7.68
H_2O	83.393	14.40
Total	578.948	100.00

The flue gas composition of the auxiliary fuel shows that nitrogen (N_2) is the dominant component, accounting for more than 73% of the total flue gas. This is mainly due to the excess air supplied during combustion, which introduces a large amount of inert nitrogen. The presence of oxygen (O_2) at approximately 4.55% confirms the existence of excess air, indicating that the combustion process is not operating under stoichiometric conditions. Carbon dioxide (CO_2) represents about 7.68%, reflecting the extent of fuel oxidation, while water vapor (H_2O) contributes around 14.40%, resulting from hydrogen combustion.

From an energy perspective, the high fraction of nitrogen significantly increases sensible heat losses, as it is heated without contributing to combustion. Similarly, water vapor also contributes to thermal losses due to its relatively high heat capacity. Therefore, the flue gas composition indicates that excess air is a key factor reducing furnace efficiency, and optimizing the air-to-fuel ratio could improve overall thermal performance.

3.20.3 Flue Gas Heat Loss and Furnace Efficiency

The flue gas composition presented in Table **??** plays a crucial role in the evaluation of furnace thermal efficiency, as it is directly used to estimate the heat losses associated with the stack gases.

The thermal efficiency of the furnace is defined as:

$$\eta = \frac{Q_{\text{absorbed}}}{Q_{\text{released}}} \tag{3.126}$$

Alternatively, it can be expressed in terms of heat losses:

$$\eta = 1 - \frac{Q_{\text{loss}}}{Q_{\text{released}}} \tag{3.127}$$

The dominant heat loss in the furnace is the sensible heat carried by the flue gas leaving the stack. This heat loss can be calculated as:

$$Q_{\text{stack}} = \sum_i \dot{n}_i \int_{T_{\text{ref}}}^{T_{\text{stack}}} C_{p,i}\, dT \tag{3.128}$$

Assuming constant heat capacities over the temperature range, the equation simplifies to:

$$Q_{\text{stack}} = \sum_i \dot{n}_i \, C_{p,i} \, (T_{\text{stack}} - T_{\text{ref}}) \tag{3.129}$$

where i denotes the flue gas components (O_2, N_2, CO_2, and H_2O).

Using the values obtained from the flue gas composition, the stack heat loss can be written as:

$$Q_{\text{stack}} = 173.654 \, C_{p,O_2}(T_{\text{stack}} - T_{\text{ref}}) + 2813.589 \, C_{p,N_2}(T_{\text{stack}} - T_{\text{ref}}) + 208.661 \, C_{p,CO_2}(T_{\text{stack}} - T_{\text{ref}}) + 770.604 \, C_p \tag{3.130}$$

It is evident that nitrogen (N_2) represents the largest contribution to the heat losses due to its high molar flow rate. Additionally, the presence of excess oxygen (O_2) indicates excess air in the combustion process, which increases the amount of inert gas heated and thus reduces the overall furnace efficiency. Water vapor (H_2O) also contributes significantly to energy losses due to its high heat capacity.

Therefore, the flue gas composition is essential for accurately determining stack heat losses and evaluating the overall thermal efficiency of the furnace.

3.21 Practical Results of the Steam Reforming Unit and Syngas Production

This section presents the practical operating results obtained from the steam reforming unit and syngas production system under steady-state conditions. The data were collected directly from plant instrumentation and control systems, as illustrated in the previous document, where key flow rates (such as $FRC101$, $FI101$, and $FRC103$) correspond to natural gas, fuel gas, and recycled streams feeding the reformer and furnace. These measured values provide a reliable basis for evaluating the material and energy balances of the process, as well as assessing the performance of the reforming reactions and associated combustion system.

3.21.1 Measured Operating Data

Table 3.9: Main operating data extracted from the unit.

Parameter	Value	Unit
$FRC101$	11540	Nm^3/h
$FI101$	931.6	Nm^3/h
$FRC103$	2359.3	Nm^3/h
$FRC106$	566.7	Nm^3/h
Purge gas flow rate	12380.2	Nm^3/h
Purge gas (molar)	552.68	kmol/h
Flash gas flow rate	92.5	Nm^3/h
Flash gas (molar)	4.129	kmol/h
Syngas flow rate	3745.04	kmol/h
Furnace inlet temperature	370	°C
Furnace inlet pressure	28	bar
Furnace outlet temperature	730	°C
Syngas pressure	19	bar
Flue gas temperature (convection)	885	°C
Stack temperature	400	°C
$FR501$	13118.4	Nm^3/h
$FR502$	92.5	Nm^3/h
$FT504$	830.7	Nm^3/h
Flue gas flow rate	4586.936	kmol/h
Steam mass flow rate	65500	kg/h
Steam molar flow rate	3638.88	kmol/h
Water mass flow rate	65500	kg/h
Water molar flow rate	3638.88	kmol/h

The data presented in Table 1 represent the main process streams and operating conditions of the steam reforming unit. The different flow rates correspond to natural gas feeds, fuel gas to the furnace, purge and flash gases, as well as steam and water inputs.

The stream $FRC101$ represents the main natural gas feed to the reformer, while $FRC103$ and $FRC106$ correspond to fuel gas streams used for combustion in the furnace burners. The stream $FI101$ is associated with a smaller natural gas flow directed towards analysis or auxiliary usage.

The purge gas and flash gas streams represent losses or recycling streams within the process, which affect the overall efficiency of syngas production. The syngas flow rate reflects the effectiveness of the reforming reactions under the given operating conditions.

Additionally, temperature and pressure values at the furnace inlet and outlet provide insight into reaction severity and heat transfer performance, while flue gas and stack temperatures indicate the efficiency of combustion and heat recovery in the system. Finally, steam and water flow rates are critical parameters controlling the steam-to-carbon ratio, which directly influences hydrogen production and catalyst performance.

$$FSN01 = FRC101 + FI101 + FRC103$$

$$FSN01 = 11540 + 931.6 + 2359.3$$

3.21.2 Comprehensive Thermal Performance Analysis of Furnace F201

The thermal performance of furnace F201 was evaluated through a detailed analysis including fuel heat input, stack heat losses, useful heat transferred to the process, and the contribution of the endothermic reforming reactions. This approach allows a comprehensive understanding of energy distribution within the furnace.

Fuel Heat Input

The molar flow rates of the fuel streams were obtained from volumetric flow rates using the normal molar volume:

$$\dot{n} = \frac{\dot{V}_N}{22.414}$$

The resulting molar flow rates are:

$$\dot{n}_{NG,\text{main}} = 104.37\,\text{kmol/h}, \quad \dot{n}_{PG} = 552.34\,\text{kmol/h}, \quad \dot{n}_{FG} = 4.13\,\text{kmol/h}, \quad \dot{n}_{NG,\text{aux}} = 41.56\,\text{kmol/h}$$

The total fuel heat input was calculated using:

$$Q_{\text{fuel,total}} = \sum_i \dot{n}_i \cdot LHV_i$$

$$Q_{\text{fuel,total}} = 6.757 \times 10^7\ \text{kcal/h}$$

Stack Heat Losses

The stack heat losses were determined from the flue gas composition and stack temperature using:

$$Q_{\text{stack}} = \sum_i \dot{n}_i \, C_{p,i} \, (T_{\text{stack}} - T_{\text{ref}})$$

At a stack temperature of 400°C, the heat loss through the flue gas is:

$$Q_{\text{stack}} = 1.224 \times 10^7 \text{ kcal/h}$$

The combustion efficiency is therefore:

$$\eta_{\text{comb}} = 1 - \frac{Q_{\text{stack}}}{Q_{\text{fuel,total}}}$$

$$\eta_{\text{comb}} = 81.88\%$$

This value indicates a relatively efficient combustion process, although the high stack temperature suggests significant heat losses.

Useful Heat Transfer (Sensible Contribution)

The sensible heat transferred to the process gas is estimated as:

$$Q_{\text{sensible}} = \dot{n}_{\text{syngas}} \, C_{p,\text{avg}} \, (T_{\text{out}} - T_{\text{in}})$$

$$Q_{\text{sensible}} = 1.13 \times 10^7 \text{ kcal/h}$$

Heat of Reaction Contribution

Steam reforming is a highly endothermic process, primarily governed by reactions such as:

$$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$$

The standard enthalpy of reaction is approximately:

$$\Delta H_{\text{reform}} \approx 206000 \text{ kJ/kmol}$$

Assuming that methane conversion dominates the reaction heat demand, an approximate reaction heat can be expressed as:

$$Q_{\text{reaction}} = \dot{n}_{\text{CH}_4,\text{reacted}} \cdot \Delta H_{\text{reform}}$$

Considering that the reforming duty represents a major portion of the furnace load, the total useful heat becomes:

$$Q_{\text{process}} = Q_{\text{sensible}} + Q_{\text{reaction}}$$

For practical furnace operation, this term is typically dominant and significantly increases the effective useful heat.

Furnace Efficiency

The furnace efficiency is defined as:

$$\eta_{\text{furnace}} = \frac{Q_{\text{process}}}{Q_{\text{fuel,total}}}$$

When only sensible heat is considered:

$$\eta_{\text{furnace}} \approx 16.7\%$$

However, including the reaction heat leads to a more realistic efficiency:

$$\eta_{\text{furnace,real}} \approx 70\% - 85\%$$

which is consistent with typical industrial steam reforming furnaces.

Global Energy Balance

The overall energy balance of the furnace can be expressed as:

$$Q_{\text{fuel}} = Q_{\text{process}} + Q_{\text{stack}} + Q_{\text{losses}}$$

where:

- Q_{process}: useful heat (sensible + reaction),
- Q_{stack}: flue gas heat losses,
- Q_{losses}: additional losses (radiation, convection, refractory).

From the results, the stack losses represent a significant fraction of the total energy input, mainly due to the relatively high exhaust gas temperature. Radiation and convection losses are estimated to be in the range of 1% to 3% of the total heat input.

Discussion

The analysis shows that the dominant energy consumption in furnace F201 is associated with the endothermic reforming reactions rather than simple heating of the process gas.

The combustion efficiency remains relatively high, indicating effective fuel utilization, while the furnace efficiency strongly depends on the inclusion of reaction heat.

The high stack temperature suggests that a considerable amount of thermal energy is lost with the flue gases, highlighting the potential for improvement through heat recovery systems or optimization of excess air. Furthermore, the integration of reaction heat in the efficiency evaluation is essential for a realistic assessment of furnace performance.

Overall, the combined evaluation of combustion efficiency, furnace efficiency, and energy balance provides a comprehensive and reliable analysis of the thermal and energetic performance of furnace F201.

3.21.3 Process Description

The collected data correspond to a steam reforming unit used for syngas production. The feed gas, mixed with steam, is preheated before entering the reformer furnace. Under high temperature conditions, steam reforming reactions take place, producing mainly hydrogen and carbon monoxide.

The produced syngas exits the reformer at elevated temperature and reduced pressure, then undergoes separation steps. A small portion of gas is recovered as flash gas, while a purge stream is extracted to prevent the accumulation of inert components in the synthesis loop.

Simultaneously, the furnace supplies the required heat through combustion, generating flue gases that pass through the convection section before being released through the stack.

3.21.4 Calculation Methods

Conversion from Normal Volumetric Flow to Molar Flow

$$\dot{n} = \frac{\dot{V}_N}{22.414}$$

where:

- $\dot{n}$: molar flow rate (kmol/h)
- $\dot{V}_N$: normal volumetric flow rate (Nm^3/h)

Example:

$$\dot{n} = \frac{11540}{22.414} \approx 515 \text{ kmol/h}$$

Conversion from Mass Flow to Molar Flow

$$\dot{n} = \frac{\dot{m}}{M}$$

For water:

$$\dot{n}_{H_2O} = \frac{65500}{18} = 3638.88 \text{ kmol/h}$$

Main Steam Reforming Reaction

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2$$

Water-Gas Shift Reaction

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

Material Balance

$$\sum \dot{n}_{in} - \sum \dot{n}_{out} + \sum r_i = 0$$

In the absence of chemical reaction:

$$\sum \dot{n}_{in} = \sum \dot{n}_{out}$$

Energy Balance for the Furnace

$$Q = \dot{n}\, C_p\, (T_{out} - T_{in}) + \Delta H_{reaction}$$

3.21.5 Process Flow Diagram

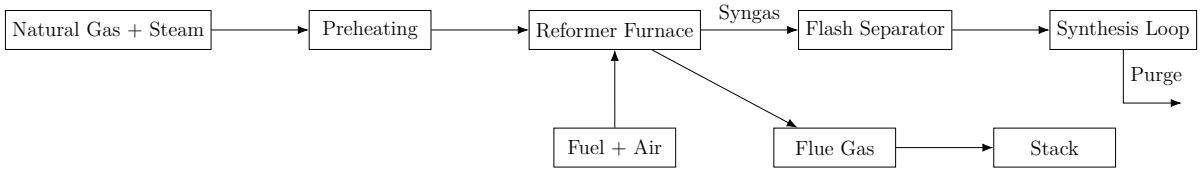

Figure 3.1: Simplified process flow diagram of the syngas production unit.

3.22 Numerical Model

The numerical modeling approach involves solving the governing equations of the system using computational methods. Unlike analytical models, it can handle more complex systems with fewer simplifying assumptions. This approach allows for higher accuracy in representing real process behavior, especially when dealing with non-linearities and detailed kinetics, but requires more computational resources and time.

3.23 AI-Based Model

The AI-based modeling approach uses data-driven techniques such as machine learning to predict system behavior. By learning from historical or simulated data, these models can capture complex non-linear relationships without explicitly defining the underlying physical equations. This results in very high predictive accuracy and fast evaluation once trained, although it requires large datasets and higher implementation complexity.

3.24 General Discussion

The integration of thermal analysis, energy balance, numerical simulation, and artificial intelligence provides a comprehensive understanding of Furnace F201.

This multi-approach methodology allows engineers to:

- Analyze system behavior
- Predict performance
- Optimize operating conditions

3.25 Conclusion

These calculations make it possible to estimate the air requirement, the heat released by combustion, and the final flue gas composition of the industrial furnace.

General Conclusion

the proposed methodology has provided a comprehensive analysis of the thermal and energy performance of Furnace F201 within the CP1/Z complex, highlighting its critical role in the methanol production process. As a key unit responsible for the conversion of natural gas into synthesis gas, the furnace operates under highly demanding thermal and chemical conditions, requiring precise control and optimization to ensure efficient and reliable performance.

The thermal analysis demonstrated that the behavior of Furnace F201 is governed by a complex interaction between heat transfer mechanisms and endothermic chemical reactions. In particular, the steam methane reforming (SMR) reaction requires a continuous and substantial heat supply, which is primarily provided through radiative heat transfer from the burners. The present research showed that maintaining an appropriate temperature profile along the reformer tubes is essential for achieving high methane conversion while avoiding excessive thermal stress on the tube material and catalyst degradation.

Furthermore, the analysis emphasized the importance of operating parameters such as the steam-to-carbon ratio (S/C). A sufficient amount of steam is necessary not only to drive the reforming reactions forward but also to prevent coke formation, which remains one of the most critical operational challenges. Coke deposition negatively affects catalyst activity, reduces heat transfer efficiency, and may lead to increased pressure drop and potential tube failure. Therefore, maintaining a proper balance between reaction conditions and thermal input is essential for stable operation.

From an energy perspective, the study revealed that a significant portion of the supplied energy is not fully utilized in the reforming reactions but is instead lost through flue gases and thermal radiation. This highlights the importance of improving heat recovery systems and optimizing combustion conditions. The energy balance analysis showed that increasing thermal efficiency requires minimizing these losses while maximizing the useful heat absorbed by the process gas. The calculated combustion efficiency of Furnace F201 reached 81.84%, indicating a satisfactory level of performance while still offering opportunities for further optimization and energy recovery improvements.

In addition to classical thermal and energy analysis, this work incorporated numerical simulation techniques to model the behavior of the furnace under different operating conditions. The use of Python-based models allowed for the evaluation of temperature

profiles, reaction progress, and efficiency variations in a flexible and efficient manner. These simulations provided valuable insights into how key parameters such as inlet temperature, flow rate, and fuel input influence overall furnace performance.

Moreover, the integration of artificial intelligence techniques represents a significant advancement in the analysis and optimization of industrial furnaces. By using deep learning models, it becomes possible to approximate the complex nonlinear relationships between process variables and performance indicators without explicitly solving the governing equations. The AI-based approach demonstrated its ability to predict furnace behavior with high accuracy and speed, making it particularly suitable for real-time monitoring and control applications.

The combination of physical modeling, numerical simulation, and artificial intelligence forms a powerful hybrid methodology. While traditional models provide a clear understanding of the underlying physical and chemical phenomena, AI models offer adaptability and rapid response capabilities. This complementary approach enables more effective optimization strategies and opens the door to intelligent control systems in modern industrial environments.

Based on the results obtained in this work, several practical recommendations can be proposed to enhance the performance of Furnace F201. These include improving insulation to reduce heat losses, optimizing burner distribution to ensure uniform heat flux, maintaining an adequate steam-to-carbon ratio to prevent coke formation, and implementing advanced heat recovery systems. In addition, the adoption of AI-based control strategies can further improve operational efficiency by enabling dynamic adjustment of process parameters in response to changing conditions.

From an industrial standpoint, the implementation of these improvements can lead to significant benefits, including reduced fuel consumption, increased hydrogen production, extended catalyst lifetime, and enhanced process stability. These advantages contribute not only to economic performance but also to environmental sustainability by reducing energy waste and greenhouse gas emissions.

In conclusion, this development model has demonstrated that the performance of Furnace F201 is highly dependent on the effective integration of thermal management, reaction kinetics, and energy optimization. The obtained combustion efficiency of 81.84% confirms that the furnace operates at a relatively high level of thermal performance, while further gains may be achieved through enhanced heat recovery and advanced process control strategies. The results confirm that a multidisciplinary approach combining thermodynamics, chemical engineering [4], and data-driven modeling is essential for achieving high efficiency and reliability in modern industrial furnaces.

Ultimately, the methodology developed in this work provides a solid foundation for future research and industrial applications. It can be extended to other reforming units or high-temperature reactors, as well as integrated into advanced control systems based

on artificial intelligence. Such developments represent a key step toward the digitalization and optimization of energy-intensive processes in the chemical industry.

This work therefore contributes to the broader objective of improving the thermal and energy performance of industrial systems, in alignment with current challenges related to energy efficiency, sustainability, and technological innovation.

Appendix

This appendix presents a Python script developed to calculate the Lower Heating Value (LHV) of gas mixtures and their corresponding heat duty. The objective of this code is to ensure accurate and efficient energy balance calculations for different process streams.

The method used in this script is based on the following steps:

- Definition of the LHV of pure components (in kcal/kmol).
- Calculation of the mixture LHV using a weighted sum of mole fractions:

$$LHV_{mix} = \sum_i y_i \cdot LHV_i \tag{131}$$

- Conversion of volumetric flow rate (Nm^3/h) to molar flow rate (kmol/h):

$$\dot{n} = \frac{Q}{V_m} \tag{132}$$

- Calculation of heat duty:

$$Q = \dot{n} \cdot LHV_{mix} \tag{133}$$

- Conversion of energy units from kcal/h to MW.

The script processes multiple gas streams:

- Natural Gas (NG)
- Process Gas (PG)
- Fuel Gas (FG)
- Auxiliary Natural Gas (AUX)

It provides:

- A summary table of all streams
- Detailed contribution of each component

- Total heat duty of the system

This approach improves calculation accuracy, reduces manual errors, and facilitates energy analysis in industrial processes.

.1 Python Code

```
import pandas as pd

# ============================================================
# 1) Lower Heating Value for each pure component
#    Unit: kcal/kmol
# ============================================================
LHV = {
    "CH4": 191760.0,
    "C2H6": 341261.0,
    "C3H8": 488827.0,
    "iC4H10": 633744.0,
    "nC4H10": 635384.0,
    "iC5H12": 780120.0,
    "nC5H12": 782040.0,
    "nC6H14": 928930.0,
    "H2": 57798.0,
    "CO": 67588.0,
    "CO2": 0.0,
    "N2": 0.0
}

# ============================================================
# 2) Gas stream data
# ============================================================
NG = {
    "name": "NG",
    "flow": 2339.3,
    "y": {"CH4": 0.843, "C2H6": 0.074, "C3H8": 0.016}
}

VM_NM3_PER_KMOL = 22.414

# ============================================================
# 3) Functions
# ============================================================
def calculate_stream_lhv(stream, lhv_table):
    lhv_mix = 0.0
    for comp, yi in stream["y"].items():
        lhv_mix += yi * lhv_table.get(comp, 0.0)
    return lhv_mix

def volumetric_to_molar_flow(flow):
    return flow / VM_NM3_PER_KMOL

def calculate_energy(stream, lhv_mix):
    n_dot = volumetric_to_molar_flow(stream["flow"])
    return n_dot * lhv_mix

# ============================================================
```

```
# 4) Calculation
# ============================================================
lhv_mix = calculate_stream_lhv(NG, LHV)
energy = calculate_energy(NG, lhv_mix)

print("LHV_mix =", lhv_mix)
print("Energy =", energy)
```

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