

The Numerical Simulation of Olefin Production Furnace for Pollution Reduction: Two case studies

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Abstract: One of the most important petrochemical processes is olefin production, and the most important part of this process is the thermal cracking furnace. The analysis of the flow and combustion process in these furnaces is important. In this research, combustion analysis in these furnaces has been investigated by examining two case studies of thermal cracking furnaces. The governing equations of the problem process, including mass and momentum and energy equations, along with combustion equations, are solved in CFX software. Temperature profiles are obtained at different points. The heat flux is obtained at different heights of the furnace. The hot spots obtained on the reactor as well as the simulation of the conversion of raw materials into products during the reactor are based on the simulation of the furnace by placing burners on the floor of the furnace (Ilam Petrochemical Olefin). Then, for the second case study, including the placement of burners in the floor and wall of the furnace (Maroon Petrochemical Olefin Furnace), thermal failure simulation has been performed. Next, optimization of combustion and reduction of Nox pollution by the re-burning method has been done.

Thermal flux is decreasing at height of more than 3 m in the furnace, which can be offset by mounting low-power burners on the wall. The excess air ratio at 1.15-0.85 has shown the best mode of reducing Nox production in the burning method.

keywords: Numerical Simulation, Furnace, Reactor, Thermal Cracking, Olefin, re-burning

1 Introduction

The thermal cracking process is one of the most important processes in the context of Olefin production. Olefin production is possible from different feeds so that countries use different feeds depending on their availability. The understanding of the critical parameters in flow and process analysis can contribute to process improvement. As such, this process has been analyzed, simulated, and optimized from different perspectives.

(Karimzadeh, Godini, and Ghashghaee 2009) proposed an algorithmic method for designing a thermal crack furnace. CFD has been used to study the efficiency and coking rate of a floor- and wall-fired naphtha furnace (Hu et al. 2011). In furnaces that are based on modern technologies, swirl flow tube

(SFT) coils are used in which efficiency is enhanced due to the swirl of the flow. Also, cracking tube surface treatments are employed to reduce coking. Efficiency can also be increased by modifying the burner structure and pattern (Zhang and Evans 2012). (Schietekat et al. 2014) analyzed these swirl coils numerically and industrially. (ZHANG, Tong, and Bingzhen 2013) used the eddy-dissipation-concept (EDC) model to explain turbulence and chemical reactions in propane cracking. (Hassan et al. 2013) employed a detailed reaction mechanism to analyze CO and NO_x emissions. A comprehensive study was conducted by Sadrameli and colleagues to review the research works on different sections of thermal cracking furnaces (Fakhroleslam and Sadrameli 2019; Sadrameli 2015). A furnace analysis has been

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performed by using the Reynolds-averaged Navier-Stokes (RANS) approach and by using the large eddy simulation (LES) method in the Open FOAM software package using the direct numerical simulations (DNS) approach (Van Cauwenberge et al. 2015). (Zheng et al. 2015) conducted 3-D combustion monitoring using 3-D observation of temperature and heat flux distribution. *Geraldine* et al. addressed the role of coatings of furnaces and tubes on increasing emissivity. They increased heat flux by 15% using high-emissivity coatings, which resulted in a 5% enhancement of the furnace efficiency in normal conditions (Heynderickx and Nozawa 2004). (Habibi, Merci, and Heynderickx 2007) dealt with the impact and comparison of radiation models in numerical simulation of the radiation inside an Olefin furnace. The researchers used a three-stage combustion model for a fuel composed of methane and hydrogen, a k- ϵ turbulence model, and P-1, Rosseland, and DO radiation models to analyze the transfer of heat and components in the furnace. The results were compared for different models, and the DO model was found to be the optimal one. A similar study was conducted by (Stefanidis et al. 2008) on the use of radiation coatings. In this case, the researchers used a non-grey gas radiation model based on the exponential wide-band model to maximize efficiency. The results reveal a 1% increase in furnace efficiency,

a 1% increase in naphtha feed conversion, and a 0.5% increase in ethylene conversion. A group of researchers in the East University of China cooperated with the Gent research laboratory in Belgium in 2011 to simulate an industrial naphtha furnace considering the radiation model and the flame length of the burners (Hu et al. 2012). (Ghasemi, Gilani, and Daryan 2016) used a case study to investigate a wall-fired furnace numerically. In another study, this research addressed the variations in the mass flow rate of the fuel in a furnace (Mohammad Ghasemi, Gilani, and Towfighi Daryan 2017). In another study, the flow inside a furnace was analyzed by the combustion chamber zoning method (Fang, Qiu, and Zhou 2017). The fouling in a furnace has also been simulated dynamically (Vandewalle et al. 2017). In addition to the thermal cracking process in the petrochemical industry, there are diverse other furnaces that have been subjected to numerical analyses by researchers depending on the topic in question (Davarpanah et al. 2019). In (Rebordinos et al. 2019) study, a numerical simulation was performed to modify a thermal cracking furnace. In recent years, the impacts of temperature on the failure of thermal cracking tubes have been explored by several researchers (Han et al. 2019). (Hu et al. 2019) employed the zone method to simulate a thermal cracking furnace.

Table 1- literature review in CFD simulation in thermal cracking furnace

No.	study	Feed	Mathematical equations	CFD	Dynamic simulation	Radiation	Convection	Reactor	Combustion	Floor burner	Wall burner	Industrial case	Nox
1	(Karimzadeh, Godini, and Ghashghaee 2009)	naphtha	*	-	*	*	*	*	-	-	-	*	-
2	(Hu et al. 2011)	naphtha	*	*	-	DO	-	*	*	*	*	*	-
3	(ZHANG, Tong, and Bingzhen 2013)	propane	*	-	-	-	-	*	-	-	-	-	-
4	(Hassan et al. 2013)	-	-	*	-	DO	-	-	*	*	-	-	*
5	(Barazandeh et al. 2015)	naphtha	*	-	*	-	-	*	-	-	-	-	-
6	(Schietekat et al. 2014)	-	-	*	*	-	-	*	-	-	-	-	-
7	(Van Cauwenberge et al. 2015)	-	-	*	-	-	-	*	-	-	-	-	-
8	(Hu et al. 2016)	-	-	*	-	Do	*	-	-	-	-	*	-
9	(Zheng et al. 2015)	naphtha											
10	(Ghasemi, Gilani, and Daryan 2016)	propane	-	*	-	Do	-	-	*	-	*	*	-
11	(Fang, Qiu, and Zhou 2017)	naphtha	-	*	-	*	-	*	*	*	-	*	-
12	(Vandewalle et al. 2017)	propane	-	*	*	-	-	*	-	-	-	-	-
13	(Mohammad Ghasemi, Gilani, and Towfighi Daryan 2017)	propane	-	*	-	Do	-	*	*	-	*	*	-
14	(Yuan et al. 2019)	naphtha	-	*	-	Do	*	-	-	-	-	*	-
15	(Rebordinos et al. 2019)	-	-	*	-	*	*	*	*	-	*	*	*
16	(Bai et al. 2019)	propane	-	*	-	-	-	*	-	-	-	-	-
17	(Hu et al. 2019)	-	*	*	-	-	-	-	-	*	-	-	-
18	This work	propane	-	*	-	Do	-	*	*	*	*	*	*

In order to compare current and past work, Table 1 lists a comparison between the research background,

including the type of feed, the type of CFD work, and how the study was conducted by different researchers.

This review of the literature shows that extensive research has focused on the simulation of reactors and thermal cracking furnaces. But, research on real cases is rare. The present research analyzes two real cases. Data are collected on the two case studies (for dimensions and processes) for the sake of 3-D modeling. Then, boundary conditions and process data are applied in the ANSYS-CFX software package to analyze and solve the governing equations numerically. After the simulation and validation, pollutant emissions and the flow inside the furnace are analyzed and the re-burning method is employed to reduce pollutant emissions in these furnaces. Also, a simultaneous analysis is performed on the furnace and reactor to produce results for the reactor products. During the modeling of the pollutants emitted from the furnace, the re-burning method is used to zone the combustion region by which any reduction in the emission of pollutants can be detected.

2 Thermal Cracking Furnace

In the studied thermal cracking process, gas is fed into the furnace and after it is cracked into smaller molecules, it is fed into the quench section. At the next step, first compression and then low-temperature cooling systems are used in the separation section to separate the products.

The furnace section that is dealt with in the present study (Figure 1) is composed of three sections including the radiation section, the convection section, and the flue section. The thermal cracking reactor is located in the radiation section where the reactions happen. Each furnace has some burners mounted at the bottom or on the wall depending on the process and feed types and the furnace process licensing company. The feed is first heated in the convection section up to a temperature that can be broken into lighter molecules in the radiation section. Various reaction mechanisms can be proposed for the conversion of the feed molecules into the product depending on the feed type. Propane is a common feed in most petrochemicals and it has been used in the present study too. Also, the present research used the mechanism introduced by (Froment, Bischoff, and De Wilde 1990) whose details are presented in Table 2.

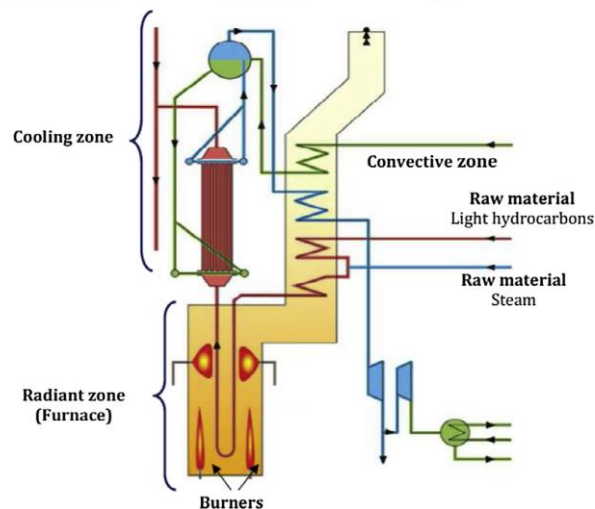


Figure 1 An overall schematic of an Olefin process furnace [7]

Table 2 The kinetics of the propane cracking (Froment, Bischoff, and De Wilde 1990)

Reaction No.	Propane cracking	A (sec ⁻¹) (k m ³ /mol.sec)	E (kJ/mol)
1	$C_3H_8 \rightarrow C_2H_4 + CH_4$	$4.692 * 10^{10}$	211.7
2	$C_3H_8 \leftrightarrow C_3H_6 + H_2$	$5.888 * 10^{10} - 9.04 * 10^5$	214.6 - 95.3
3	$C_3H_8 + C_2H_4 \rightarrow C_2H_6 + C_3H_6$	$2.536 * 10^{13}$	247.1
4	$2C_3H_6 \rightarrow 3C_2H_4$	$1.514 * 10^{11}$	233.5
5	$2C_2H_6 \rightarrow 3CH_4 + 0.5C_6$	$1.423 * 10^9$	190.4
6	$C_3H_6 \leftrightarrow CH_4 + C_2H_2$	$3.794 * 10^{11} - 2.32 * 10^7$	248.5 - 123.7
7	$C_2H_6 + C_3H_6 \rightarrow CH_4 + C_4H_8$	$5.553 * 10^{14}$	251.1
8	$C_2H_6 \leftrightarrow C_2H_4 + CH_4$	$4.652 * 10^{13} - 9.97 * 10^8$	272.8 - 138.0
9	$C_2H_4 + C_2H_2 \rightarrow C_4H_6$	$1.026 * 10^{12}$	172.6

3 The Governing Equations

3.1 Equations of mass and energy conservation

The mass conservation equation, or the continuity equation, can be written as below

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_m \quad (1)$$

Eq. (1) is the overall form of the mass conservation equation used for both compressible and incompressible flows. The source term S_m is the mass added to the continuous phase from the second phase (e.g. due to the evaporation of liquid drops).

The momentum conservation in the i direction in an acceleration-free control volume is as below:

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i \quad (2)$$

In which the stress tensor τ_{ij} is as below:

$$\tau_{ij} = \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_i} \delta_{ij} \quad (3)$$

The second term in the right-hand side of the equation shows the stress induced by a change in the element volume.

The energy equation is as below in its general form:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_i} \left(K_{eff} \frac{\partial T}{\partial x_i} - \sum_j h_j J_j + u_j (\tau_{ij})_{eff} \right) + S_h \quad (4)$$

in which K_{eff} is the effective coefficient of conductivity defined as $k_{eff} = (k + k_t)$ in which k_t represents turbulent heat conductivity coefficient based on the applied turbulence model and J_j is the diffusion flux of the j' component. S_h includes the heat of the chemical reaction and any other volumetric heat sources defined. In this equation, we have

$$E = h - \frac{p}{\rho} + \frac{u_i^2}{2} \quad (5)$$

so that h for an ideal gas is

$$h = \sum_{j'} m_{j'} h_{j'} \quad (6)$$

in which $m_{j'}$ is the volumetric fraction of the j' component and $\int_{T_{ref}}^T c_{p,j'} dt$ and $T_{ref} = 298/5 \text{ K}$.

3.2 The radiation models in calculating heat transfer

There are various radiation models for numerical solvers. Based on the history and trend of solvers, the present study uses the DO method (Habibi, Merci, and Heynderickx 2007).

3.3 Components transfer equations and turbulent flow modeling

The K- ϵ turbulence model is used to solve this problem, and the equations of the components transfer are selected from the literature, which is not mentioned here to save in space (Heynderickx and Nozawa 2004).

3.4 Discretization of equations and boundary conditions

The integral equations governing the problem, including mass, momentum, and energy conservation equations, components transfer equations, and turbulence equations, are solved by the finite volume method as described below:

- Dividing the solution range into separate criterion volumes using a computational network
- Integrating the governing equations over the individual criterion volumes to form algebraic equations in order to determine the dependent variables, e.g. speed, pressure, temperature, and scalar variables
- Linearizing discrete equations and solving the derived linear equations system to determine the new values of the dependent variables

3.5 Sequence of steps and solution procedure

The problem is solved by the coupled solution method in the ANSYS-CFX software package. In this method, the governing equations are solved simultaneously. Since the governing equations are nonlinear, several iterations of the solution loop are required to reach convergence. The solution flowchart is as below for each iteration and each step.

1. Select flow properties. (If this is the first step of solution, use the initial conditions, but if it is iteration, use the results of previous iterations.)
2. Solve the momentum equations u , v , and w using the current values for pressure and mass fluxes to find the speed field.
3. Since the speeds obtained in the first step may satisfy the continuity equations locally, derive a Poisson-type equation to modify pressure in continuity equation and linearized momentum equations. Then, solve the modified pressure equation to obtain modifications required for pressure and speed fields and mass fluxes so that the continuity equation is satisfied.
4. Solve the equations of scalar variables, e.g., turbulence, energy, and chemical components, by the values obtained for the other variables.
5. Control the convergence of the equation.

These steps go on as long as the convergence is satisfied.

4 Generation of Geometry and Meshing

4.1 The bottom-fired furnace of Ilam Petrochemical Complex

The Olefin unit of the Ilam Petrochemical Complex has four furnaces, each with two cells. Each cell has 24 coils. Here, we explored two head-to-head coils. The furnace height at the radiation part is 10.5 m, its width is 3 m, and its studied depth is 1.5 m. Table 3 shows the specifications of this furnace.

Table 3. The specifications of the furnace and reactor in the Ilam Petrochemical Complex

Furnace dimensions and specifications		Reactor specifications	
Length (m)	1.5	External diameter (mm)	77.5
Width (m)	3	Internal diameter (mm)	63.5
Height (m)	10.5	Length (m)	40.5
Number of burners	2	Number of passes	2

The first step of numerical simulation is the production of geometry. The development of geometry and computational network is among the most important and time-consuming parts of numerical analyses. The geometry was developed by the Gambit and SolidWorks software packages. Figure 2 depicts the geometry developed for the Ilam furnace.

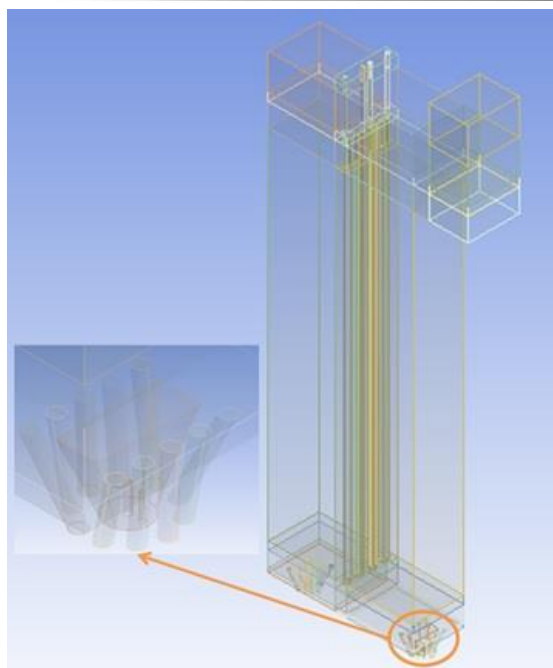


Figure 2. The geometry of the Ilam furnace

4.2 The bottom- and wall-fired furnace of Maroon Petrochemical Complex

The solution method in this section is similar to the modeling of the Ilam furnace. The software for geometry development and solver is also similar to the previous section, and the solution geometry is just changed. Figure 3 shows the geometry and meshing of the Marun furnace.

4.3 Boundary conditions

4.3.1 Boundary conditions of walls

In most cases, the CFX software considers the default values. In this problem, the boundary condition of a slide-less wall with no mass flux of the chemical components, no movement, and no separation of the phases and adiabatic conditions for the wall is applied. The radiation applied to the walls is considered to be opaque. The emissivity is assumed to be 0.85 for the furnace wall and 0.6 for the tubes.

4.3.2 Inlet boundary condition

In this problem, since the mass flow rate of the fuel and air is known at the inlet duct of the burners, the boundary condition for the inlet mass flow is selected for these inlet ducts. The data required to apply this condition are as below.

Since the mass flow rate is known, this condition is used in the boundaries for different ducts. The direction of the inlet flows is selected to be perpendicular to the boundary surface. The method of calculating disturbance at the inlet boundaries is selected to be medium (5% intensity) and the flow is complete. Since the inlet ducts of fuel and air are separate and the burner is modeled as diffusion, the mass fractions of the chemical components for the inlet ducts of the fuel and air are known.

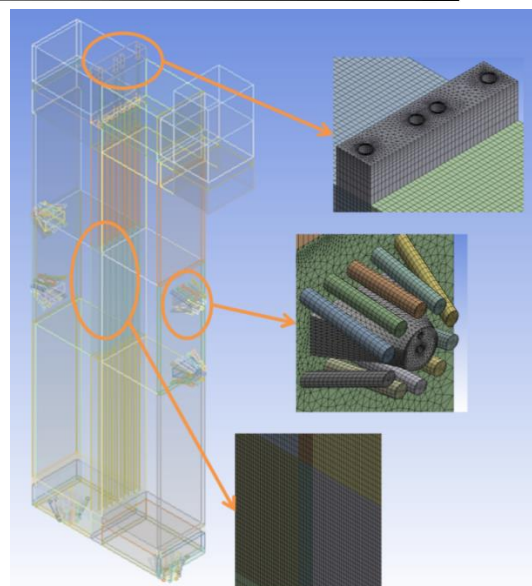


Figure 3. The production network in the Maroon furnace

(The mass fraction of methane (CH_4) is 1 for the fuel inlet duct and 0 for the rest, and the mass fractions of oxygen (O_2) and nitrogen are 21% and 79% for the air inlet duct, respectively).

The inlet flows are selected to be perpendicular to the boundary surface. The method of calculating disturbance in the inlet boundaries is assumed to be medium (5% intensity) and the flow is complete. Also, it is assumed that the feed provided to the tubes is pure propane (100% mass fraction of propane). Tables 4 and 5 present the boundary conditions applied at the inlet ducts of the burners and tubes.

Table 4. The boundary conditions applied at the burner inlet

Fuel mass flow rate	173 kg/hr
Air mass flow rate	4320 kg/h
Primary air percentage	20%
Secondary air percentage	80%
Inlet air temperature	25°C
Fuel temperature	15°C

Table 5. Boundary conditions at the inlet of tubes

Total inlet pressure	206 kPa
Feed inlet temperature	873 K

4.3.3 External boundary conditions

The mass flow rate and composition of the combustion gases are unknown at the outlet duct of these gases to the environment, so the outlet mass flow condition cannot be used. But, the pressure is known at the outlet. Thus, the outlet pressure boundary condition is used for this duct. To use the outlet pressure condition (for gases outlet duct), the static pressure should be known at the outlet. The outlet static pressure is assumed to be atmospheric pressure.

4.3.4 Periodic boundary condition

Each node and element on one of the periodic surfaces

is linked to its corresponding node and element on the opposite-side periodic surface so that when solving, the Navier–Stokes, and energy equations are solved only for one of them and the result is considered for both elements. In other words, the nodes and elements on the periodic surface are in the form of pairs with identical flow properties. The flux on the element surfaces in the periodic boundaries is so calculated that the outlet flux of the periodic boundary elements is equal to the inlet flux of its corresponding surface in the corresponding elements on the other periodic surface. As was already mentioned, the periodic boundary condition has been applied to avoid the redundant increase in the number of computational elements.

4.3.5 Interface boundary condition

Finally, the solid zone (the thickness of the reactor tubes) should be defined as an interface. To this end, two boundary conditions of interface and solid-fluid should be defined – one between the fluid inside the tubes and the solid zone and the other between the fluid inside the furnace and the solid zone.

5 Results

5.1 Thermal properties

Here, we first analyze and compare the results of real geometry data with simultaneous modeling and numerical simulation of the furnace and thermal cracking reactor. For simulation, the design conditions of the Olefin furnace at the Ilam Petrochemical Complex have been employed. Then, the effect of the re-burn method is explored on reducing NO_x emission through modeling the Olefin furnace at the Maron Petrochemical Complex

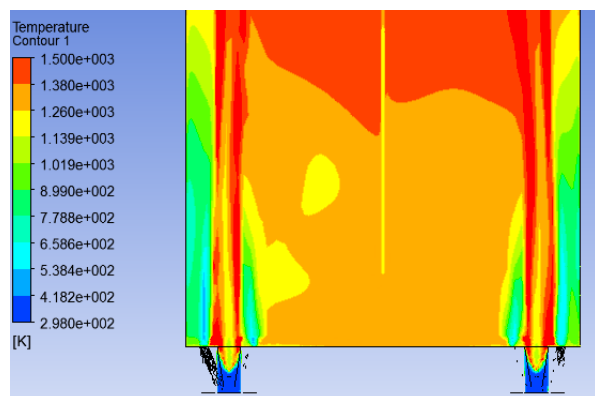


Figure 4. Flame at the vertical cross-section of the furnace

Figure 4 displays the temperature counter at the vertical cross-section of the furnace. The flame has a proportional shape. It terminates at a height of about 6 m, after which we approach thermal uniformity. Also, the flame has been formed at a good distance from the middle part of the furnace where the reactor tubes are located. So, the tubes are not exposed to high pressure. Also, the tubes are not in direct contact with the flame, so they are not at the risk of burning.

Figure 5 depicts the variations in gas temperature

in terms of the in-furnace height. It is observed that the temperature variation trend matches the laboratory documents. However, there is some error in the calculation, which is inherent to all computational works.

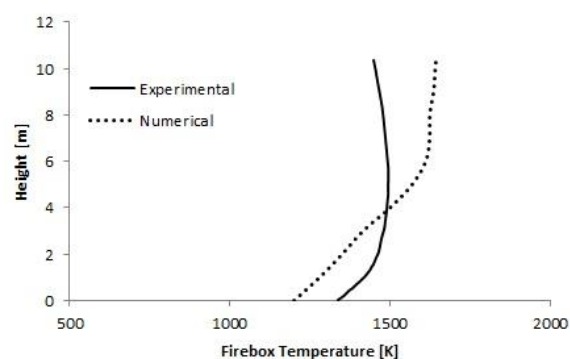


Figure 5. The graph of the mean temperature of in-furnace combustion gases

The comparison in this figure shows that the greatest error in the results of modeling compared to the actual results is 13%, which can be regarded as an acceptable error for the following reasons.

Table 6. A comparison between the industrial and computational results for the outlet temperature of the radiation box

Outlet temperature of the box (Numerical)	Outlet temperature of the box (Industrial)	Difference (%)
1390°C	1127°C	19

Table 7. A comparison between the industrial results for NO_x and the numerical analysis

NO_x (Numerical)	NO_x (Industrial)	Difference (%)
65.45 ppmv	58.44 ppmv	11.99

Numerical computations are subject to errors from various sources. The main source in our modeling is related to the geometry modeling, merely resulting from the unavailability of accurate industrial documents. A key reason for the error in the results is the lack of access to the precise geometry of the burner's fuel nozzles. Consequently, we could not access the precise profile of the outlet gas flow of the burner. Also, neglecting the swirl of the inlet airflow of the furnace has adversely affected the modeling. Since swirl fins were not built in the burner geometry, the mixing process of the air and fuel does not exactly match the reality. The modeling has been subject to other sources of errors, e.g., approximations that were not considered in the calculations, but the two abovementioned reasons were the key ones.

Now that we compared the modeling results with real data and verified the numerical results, the results depicted in the figures are discussed. Figure 6 displays the flow field formed inside the furnace. The distribution of the gas flow rate at the top of the burners is not perfectly symmetrical. This is related to

the fact that the outlet of the gas flow is located on one side of the furnace. At the top of the furnace, the gases on the other side should also leave the furnace and this causes asymmetry of the speed field. Also, large zones of returning flows are observed around the tubes, which are related to the very high rate of the outlet gases of the burners. The gas flow rate gradually slows down. Overall, the total gradient of the rate will be small due to the returning flow, and the penetration and mixture of the gases on both sides of the tubes. This figure also shows the returning flows at the top of the furnace and the bottom parts of the gas outlet duct. On the right-hand corner of the figure, the returning flows result from the separation of the flow from the wall, which leads to the separation of the boundary layer. This is caused by the tendency of the gas to leaving from the other side of the furnace. The returning flows in the outlet part are also caused by the 90° turning of the direction, which happens at the high gas rate.

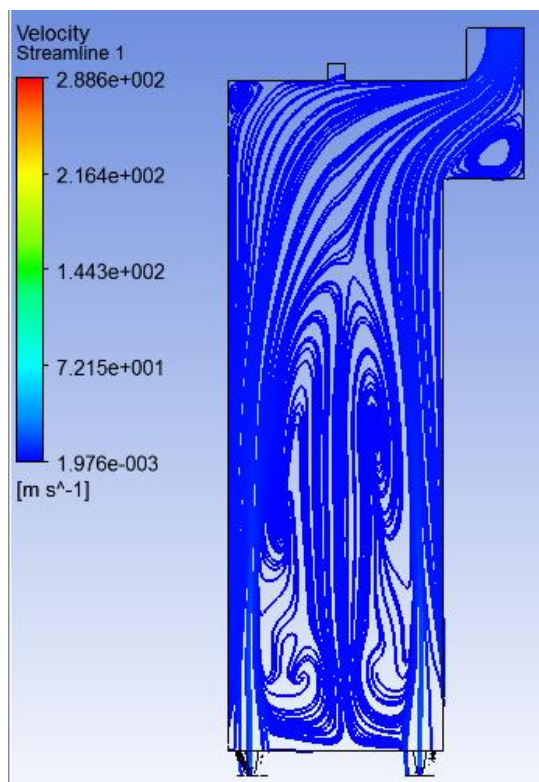


Figure 6. The lines of gas flow inside the furnace

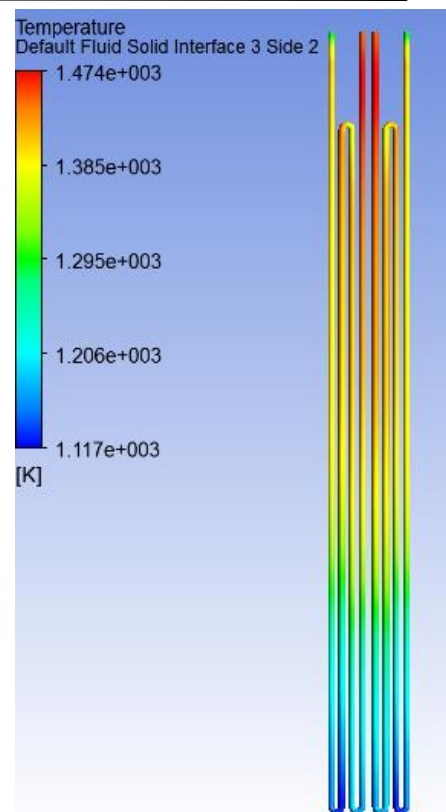


Figure 7. The temperature contour for the tube surfaces

An issue that should be discussed is the surface temperature of the tubes since it is important as a boundary condition in determining the rate of heat transfer into the tubes. Figure 7 shows the temperature counter of the tube surfaces. It is observed that the temperature is minimal at the bottom of the furnace where the flame has not maximized yet, but it is maximal at the upper parts that are exposed to hotter gases. This temperature contour will be discussed more below along with the profile of in-tube feed temperature variations.

Figure 8 depicts the temperature contour at the traverse section of the furnace and the upper parts, i.e., the outlet of combustion gases. It is inferred from the figure that the temperature around the tubes is higher than the temperature of their surface, implying the driving force of heat transfer into the tubes. This is true for the whole height of the furnace. In support of this explanation for Figure 8, the temperature of the furnace walls is higher than the temperature around the tubes.

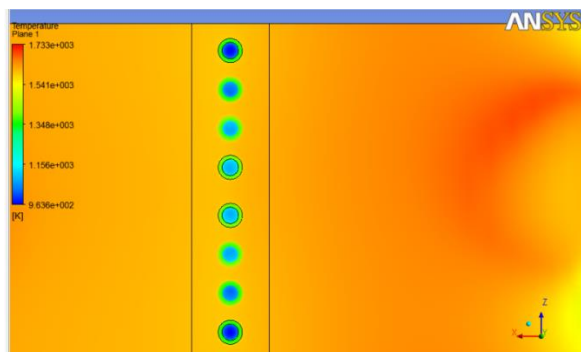


Figure 8. The temperature contour at the outlet of the combustion gases

5.2 Concentration of components

After analyzing the results on temperature and heat transfer, we now discuss the results on the concentration of components in the furnace and the weight percentage of the products and raw material

along the reactor.

We first examine the concentration of methane, which has been used as fuel. As is evident in Figure 9, the methane concentration is the highest at the fuel inlet zone. As one rises along with the flame, its concentration goes down until it almost reaches zero at the top of the furnace. Figure 10 shows the concentrations of CO_2 at the fuel inlet zone and around the flame. Expectedly, it is zero at the beginning and the inlet of the flame, but CO_2 is generated around the flame due to the combustion.

Since the methane burning process is defined as a single-step reaction in which it is converted into CO_2 , the CO concentration is zero all inside the furnace. Since the counter of the steam concentration is similar to that of CO_2 , it is not shown.

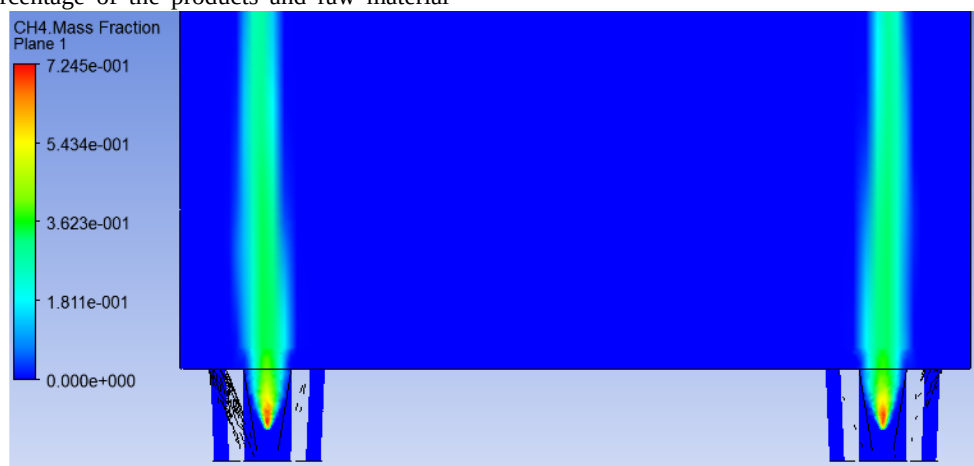


Figure 9. The concentration of methane at the inlet and around the flame

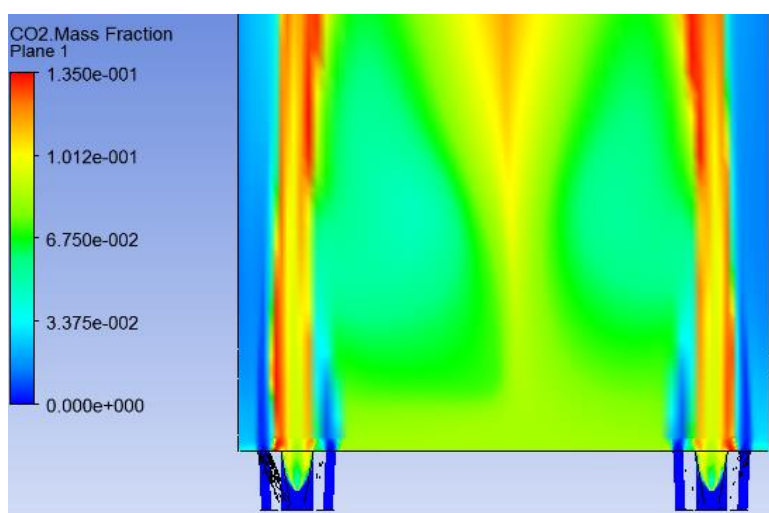


Figure 10. The weight percentage of CO_2 around the flame

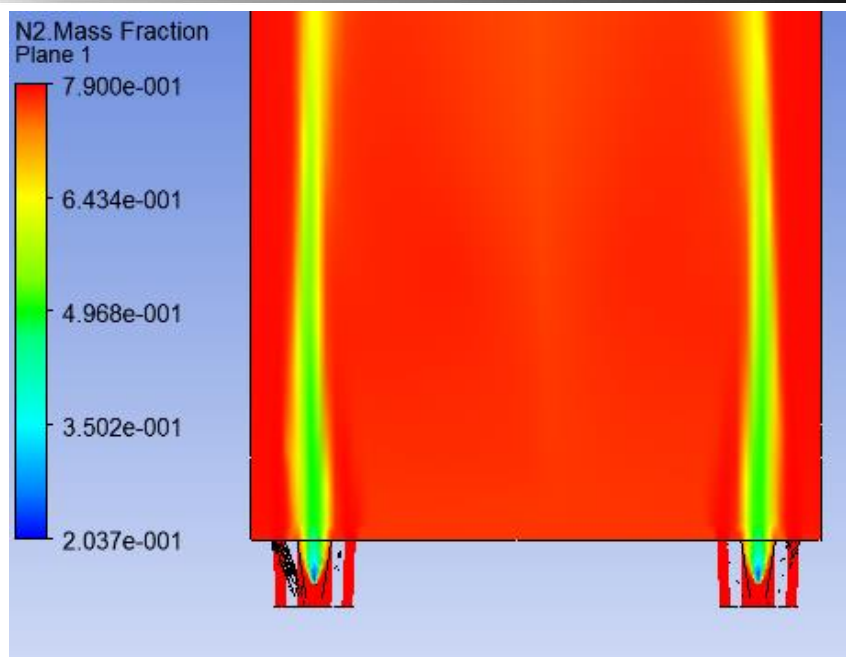


Figure 11. The weight percentage of N around the flame

It is observed in Figure 11 that the concentration of N as an inert gas is 79% at the air inlet. If NO_x production is considered, this profile will change slightly. Also, the concentration of N is seen to be very low around the flame. According to Figure 12, the concentration of oxygen as a consumption element is 11% at the air inlet and about zero around the flame.

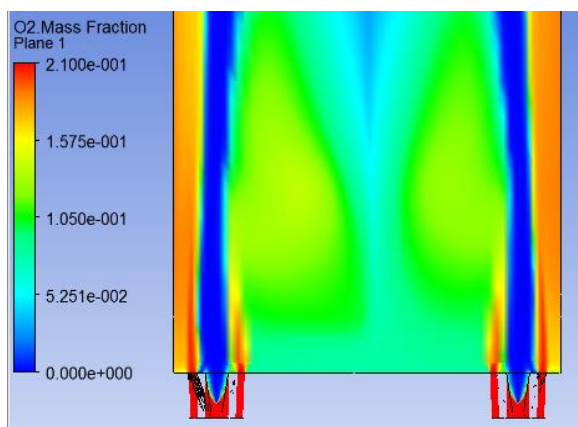


Figure 12. The weight percentage of oxygen at the air inlet and around the flame

Figure 13 shows the counter of the total pressure around the flame. It is seen that the total pressure is higher in the parts that the gas is sucked into the furnace swiftly than inside the furnace. The maximum total pressure is observed in the fuel nozzle part.

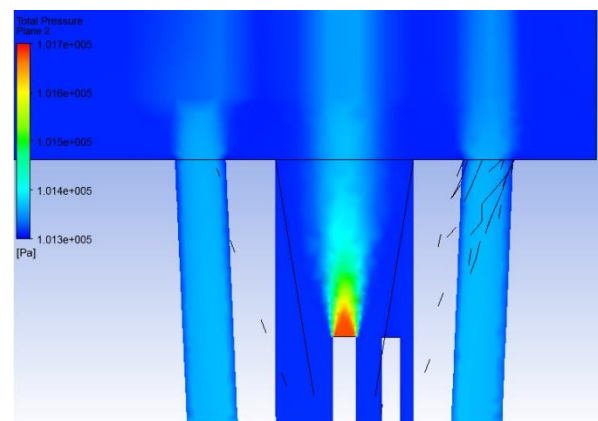


Figure 13. The pressure inside the furnace and around the flame

After the concentration of the components inside the furnace is checked, data on the concentration of feed and products along the reactor are now presented. The feed is pure propane that is sent into the tubes under the condition of inlet pressure and is converted into the product and other byproducts along the path by thermal cracking. The figures shown below reveal that the concentration of propane decreases as it passes through the reactor tubes, but in contrast, the concentration of the desired products, e.g., ethylene and propylene, start to increase as one moves along the tubes.

Figure 14 shows the variations in the weight percentage of propane, which formed the feed. First, it shows a slow decline, but it speeds up as the temperature increases and this trend sustains until it leaves the tubes. Figure 15 displays the variations in the weight percentage of ethylene. The weight percentage of this product first increases slowly, which is related to the low temperature of the feed

gas. At the end of the first pass, where the temperature of the feed inside the tubes further increases, more and more ethylene is produced. When the feed gas enters the outlet tube, the weight percentage of ethylene slowly increases due to the decline in reactants.

In Figure 15, the variations in propylene weight percentage are depicted. The increasing rate of this product is slow at first, but it increases faster in the middle of the reactors. Finally, as the weight percentage increases and the feed temperature inside the tubes go up, some extra reactions happen during which this product is used to produce such byproducts as CH_4 and C_2H_4 . Consequently, the net rate of propylene production decreases at the end of the reactor.

Figures 16 and 17 illustrate the weight percentage of two other products, i.e., methane and hydrogen. The mass ratios of these two products are lower than that of the optimal products and they are produced by some extra reactions.

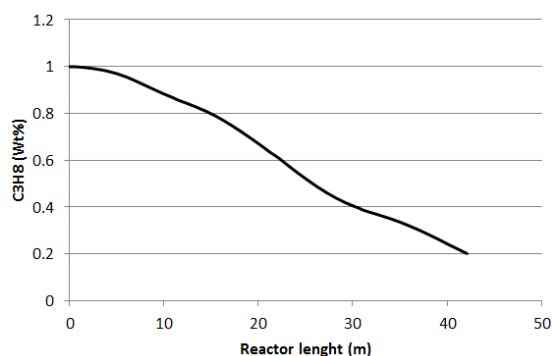


Figure 14. The weight percentage of propane along the reactor

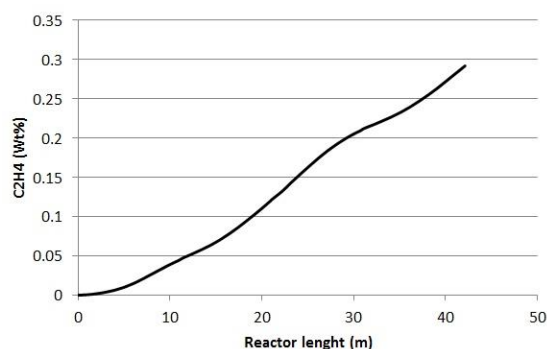


Figure 15. The weight percentage of ethylene along the reactor

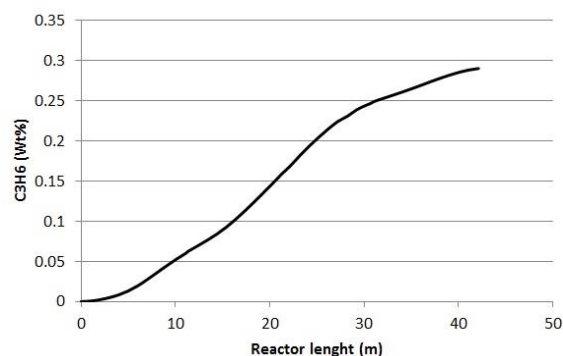


Figure 16. The weight percentage of propylene along the reactor

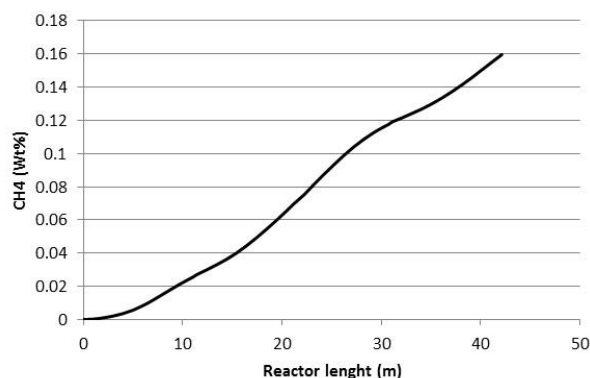


Figure 17. The weight percentage of methane along the reactor

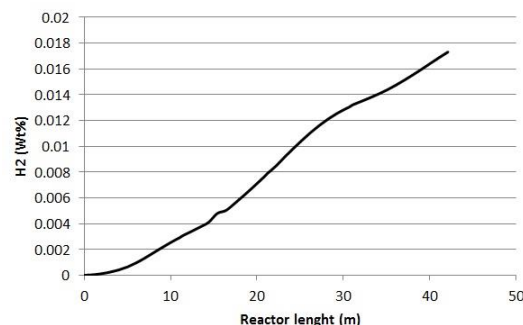


Figure 18. The weight percentage of hydrogen along the reactor

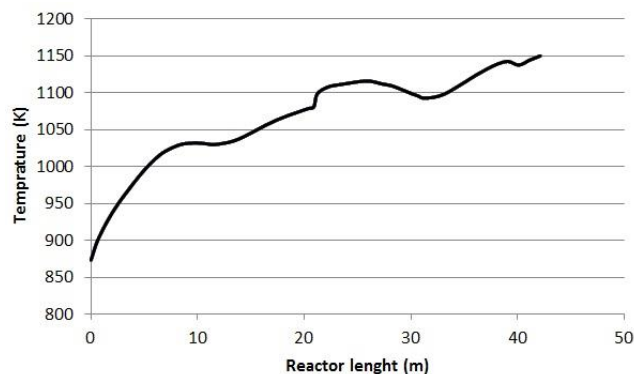


Figure 19. The temperature of propane along the reactor

Figure 19, shows the plotting of the feed

temperature inside the tubes in terms of the tube length. The comparison of this figure and the temperature counters shown in the above figures allows studying the trend observed in the figure on the temperature contour. It is observed that the temperature graph has two relative minimums at the lower bends, which is related to the low temperature of the flame at this point. Additionally, two maximum points are observed in the graph, which can be observed and matched by referring to the temperature contour on the tubes.

This means that the feed temperature inside the tubes starts to rise from the very beginning, and its temperature profile will have maximum and minimum points due to the temperature variations of the gases around the tubes.

Furthermore, based on Figure 19, the comparison of the temperature between the tube surface and feed at different points reveals the temperature difference. This difference is responsible for the establishment of heat transfer between the tube and the feed inside the tube. The potential required for heat transfer is observed in this temperature difference.

Figure 7 compares the outlet temperature of the furnace products with the product outlet temperature obtained from the numerical simulation.

Table 8. A comparison between the industrial and numerical results for the outlet temperature of the products

Outlet temperature of products (Industrial)	Outlet temperature of products (Numerical)
857°C	877.11°C

6 Optimization of furnace pollutants by the re-burning method

Here, we focus on the thermal cracking furnace in the Maron Petrochemical Complex. The difference between this furnace and the furnace of the Ilam Petrochemical Complex is that it is wall-fired. Wall-fired furnaces have not only higher thermal efficiency and more uniform distribution of temperature along with the furnace, but they can also be effective in reducing furnace pollutants.

It is well-known that an effective way to curb NO_x emission is the use of the re-burning method by which NO_x emission is significantly reduced by combustion localization. Here, we first explain the re-burning method briefly. Then, the target furnace will be modeled.

6.1 Re-burning method

The re-burning method is principally based on modifying the combustion system. In this method, the combustion zone is divided into two sections. In the first section, the ratio of fuel to air increases in the burners, thereby creating a fuel-rich zone when compared to the stoichiometric mode. In this zone, since there is oxygen deficiency due to the lower amount of air, a part of the hydrocarbons of the fuel go to the next section unreacted and unburned. In this zone, the flame's adiabatic temperature decreases

because of exiting from the stoichiometric mode. The combustion gases go through the fuel-rich zone and enter the fuel-poor zone where the ratio of fuel to air in the burners is lower than that of the stoichiometric mode. Consequently, oxygen is increased in this zone, and as a result, the hydrocarbons left unburned in the previous section are burned, and the thermal power requirement is supplied.

6.1.1 Fuel-rich zone

As was explained, the adiabatic temperature of the flame is lower in the fuel-rich zone than in the stoichiometric mode. A key factor in NO_x emission is the adiabatic temperature of the flame. Since the reactions leading to NO_x emission are active in the temperature range of 1500-2100 K, i.e., this is the optimal range for NO_x emission, so to reduce NO_x emission, this thermal range should be avoided from happening. This realizes in the fuel-rich zone due to the decline in the flame's adiabatic temperature. Another factor that is effective in reducing NO_x emission in this zone is the lower amount of oxygen and nitrogen compared to the stoichiometric mode and the decline in the collision of their molecules, which results in lower NO_x emission. Therefore, NO_x emission will decrease in the fuel-rich zone. However, its produced thermal power will be lower due to incomplete combustion.

6.1.2 Fuel-poor zone

In this region, since the ratio of fuel to air is lower in the burners, the flame's adiabatic temperature cannot rise and remains at a level lower than the optimal temperature range for NO_x emission. As such, although the amount of oxygen and nitrogen, as well as collisions, are increased in the fuel-poor zone, NO_x emission is decreased remarkably due to exiting from the optimal temperature window. In addition, since unburned carbons left from the previous section are burned in this zone, the thermal power requirement is supplied.

6.1.3 Effects of using the re-burning system

As a result of modifying the combustion system by the re-burning method, the total NO_x emission of the two stages is reduced significantly. However, this method slightly reduces thermal power and CO production because the concentration of oxygen is low in the fuel-rich zone. We know that oxygen radicals (O) are required to produce CO molecules, whereas O_2 molecules are required for the formation of CO_2 molecules. So, CO production is increased in this zone. On the contrary, the rate of CO_2 production is increased in the fuel-poor zone due to the higher concentration of oxygen versus the previous section and the stoichiometric mode as well as the more stability of CO_2 molecules versus CO molecules.

Overall, the consequences of the re-burning method can be summarized as below:

1. A decrease in NO_x emission
2. An increase in the number of unburned hydrocarbons
3. A slight decrease in the produced thermal power
4. An increase in CO_2 production
5. A decrease in flame temperature, and consequently, a decrease in temperature at all points inside the furnace

6.2 Effects of the re-burning cases

To examine the effect of using the re-burning method on NO_x reduction, seven cases are defined for different combustion values, as listed in Table 9. Then, they are separately modeled, and the results are derived. As was already mentioned, the burners are divided into two sections, including fuel-rich and fuel-poor zones in the re-burning method. The air-fuel ratio is higher in the fuel-rich zone than in the stoichiometric state. First, the stoichiometric state should be modeling to provide a criterion for exploring the use of the re-burning method. Then, the other cases should be modeling by making changes in the balance ratios.

When simulating, the balance ratios are changed in the burners to create the different cases of fuel-rich and fuel-poor conditions in the burners, and the NO_x emission is then estimated. It should be noted that the balance ratio is changed only by changing the mass rate of the air, and the fuel rate is not changed since the power is constant. To apply the changes, the burners should be assigned to the two zones. The fuel-rich zone is created by the bottom-mounted burners, and the fuel-poor zone is created by the wall-mounted burners.

Table 9. The balance ratios applied in different runs of the problem

Cases	Fuel-rich zone	Fuel-poor zone
Case 1: Stoichiometric state	1.000	1.000
Case 2	1.050	0.950
Case 3	1.100	0.900
Case 4	1.150	0.850
Case 5	1.200	0.800
Case 6	1.250	0.750
Case 7	1.300	0.700

Table 10 shows the rate of NO_x emission in different combustion cases. The stoichiometric state has the highest rate, but as the balance ratios are changed, NO_x emission is reduced in all cases versus the stoichiometric state. But, the trend is not linear, and no special regularity can be detected.

Figure 20 depicts NO_x distribution inside the furnace in the stoichiometric state of combustion. NO_x is the densest between the bottom burners and wall burners because combustion in the bottom burners happens with no extra air and the pollutant emissions are much higher than the optimal level. The results also indicate that the NO_x emission rate is much higher in the stoichiometric case than in other cases.

Table 10. The rate of NO_x emission in different cases

Cases	NO_x formation (ppm)	NO_x reduction (%)
Case 1: Stoichiometric state	680.9692	0
Case 2	255.3252	62.50731
Case 3	115.1468	83.09151
Case 4	125.8827	81.51502
Case 5	119.6575	82.42914
Case 6	182.61	73.18502
Case 7	134.0004	80.32299

Figure 21(a-f) displays the NO_x distribution in different combustion cases, evidently demonstrating a decline in NO_x emission. This decline can be readily observed by comparing the counters in Figure 21(a-f) with those in Figure 20. This reduction is directly associated with the impact of the re-burning method and the changes applied in the combustion conditions. The results in Figure 21(a-f) show the rate of NO_x emission during the combustion process.

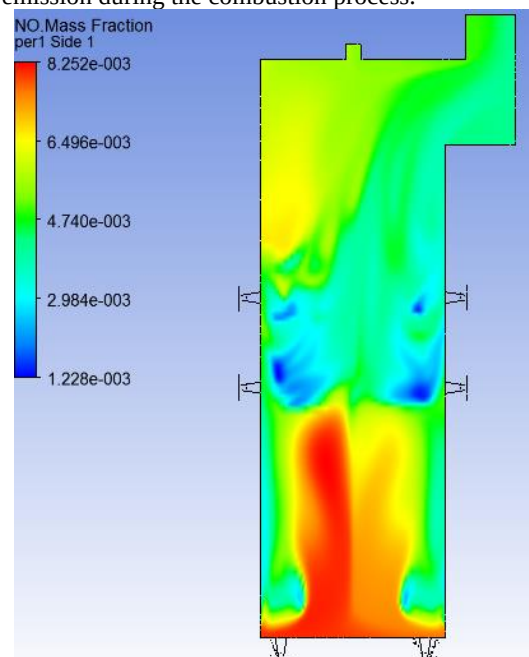
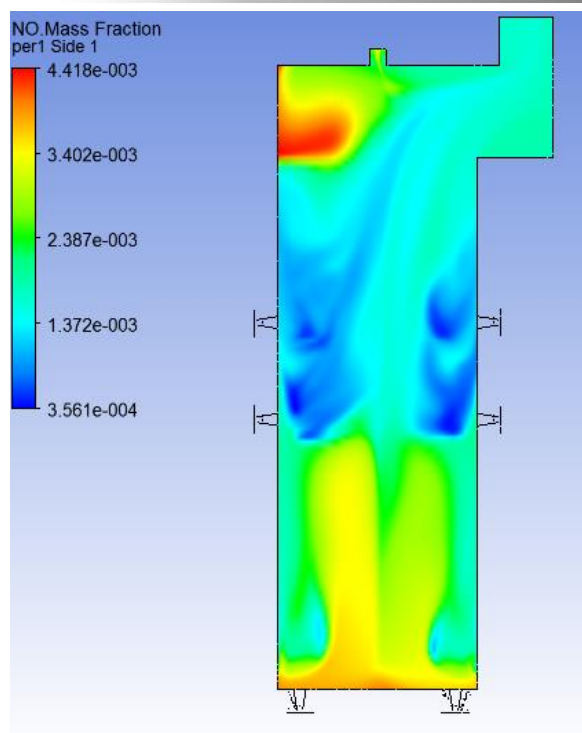
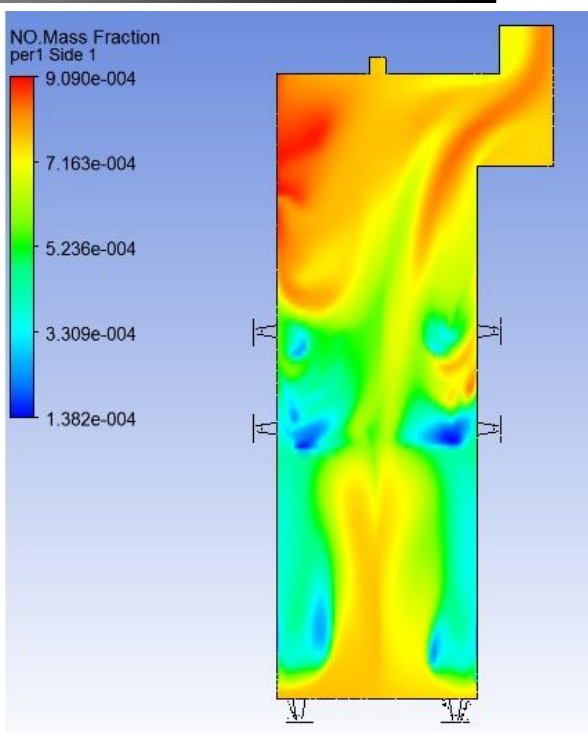


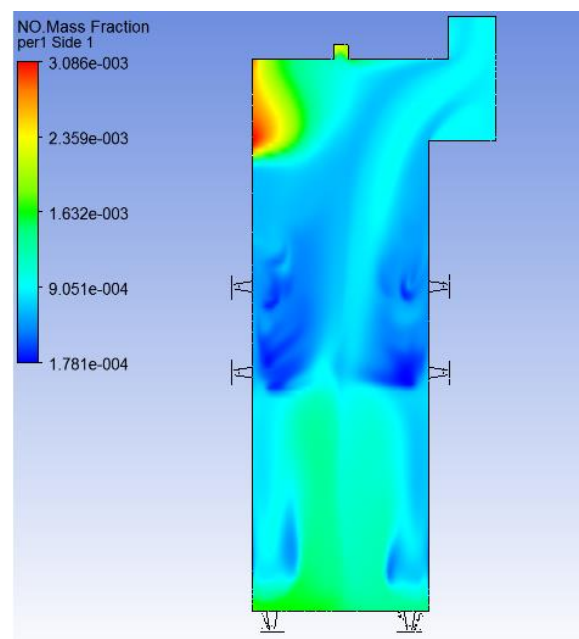
Figure 20. The distribution of NO_x inside the furnace at the stoichiometric state



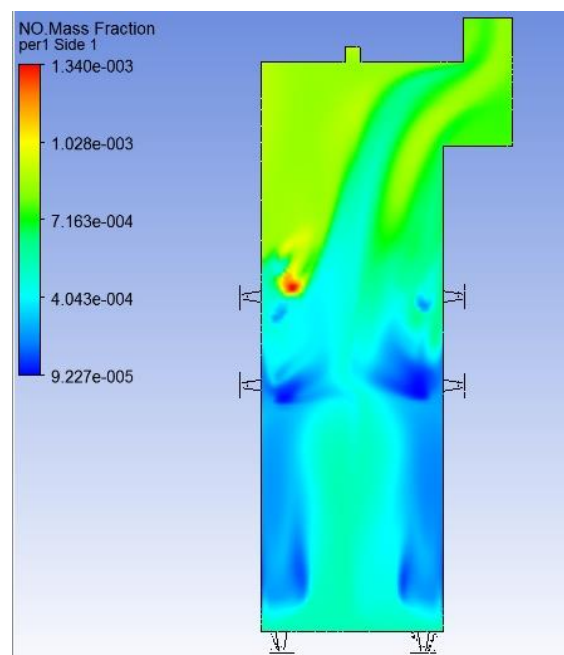
(a) Case 2



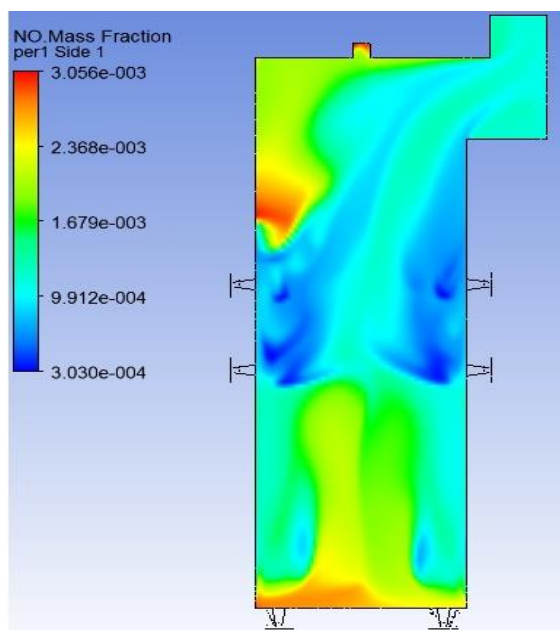
(b) Case 3



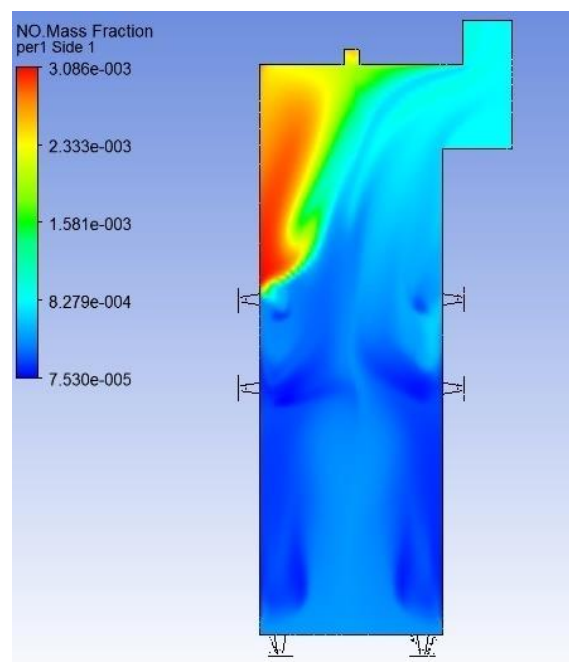
(c) Case 4



(d) Case 5



(e) Case 6



(f) Case 7

Figure 21. The distribution of NO_x inside the furnace at different cases studied here

The fuel-rich combustion at the lower levels of the furnace results in the generation of some unburned hydrocarbons that have had no chance to burn due to oxygen deficiency. Although a great part of these hydrocarbons reacts with oxygen and burns in the upper levels, a part exits the furnace completely unburned. In the re-burning method, if one aims to establish optimal balance ratios to reduce NO_x emission, a number of unburned hydrocarbons will be unavoidable. This is observed in Table 10.

Table 11 presents the rate of unburned hydrocarbons during the combustion process and the percent increase in its concentration at different combustion cases versus the stoichiometric case. It is seen that the highest increase in CH₄ happens in Cases 4 and 5 in which the decline in NO_x emission is the greatest. This ascending trend of completely unburned hydrocarbons is consistent with what was already mentioned about the consequences of the re-burning method.

Table 11. The amount of unburned CH₄ at different combustion cases

Cases	Unburned CH ₄ (mass fraction)	Unburned CH ₄ (increase %)
Case 1: Stoichiometric state	0.005506	0
Case 2	0.008329	51.2746
Case 3	0.008623	56.6073
Case 4	0.010914	98.2201
Case 5	0.010955	98.9666
Case 6	0.010721	94.7149
Case 7	0.010697	94.2735

The distribution of the unburned hydrocarbons, which is only CH₄ here, is shown in Figure 22. The figure displays the distribution for the stoichiometric

state. It is observed that this concentration is in total negligible, and it is higher around the flame than in other zones. The other combustion cases are not shown.

It is evident in these figures that a great part of the unburned hydrocarbons is in the fuel-rich zone, i.e., around the flames of the bottom burners. This increase is related to the decline in the ratio of air to fuel in this zone and the increase in the hydrocarbon contents versus the stoichiometric case, which is evident in these figures.

The rate of CO₂ production is increased in the re-burning method since the combustion is not stoichiometric and the amount of unburned hydrocarbons is greater. The distribution of CO₂ inside the furnace (Figure 23) shows that CO₂ is mostly produced by the conversion of CO to CO₂, and this happens in zones higher than the wall burners. This can be ascribed to the higher concentration of oxygen in the fuel-poor zone versus the stoichiometric case and the higher stability of CO₂ molecules versus CO molecules.

A product of combustion is water generated by the reaction of hydrogen with oxygen at high temperatures. The rate of H₂O production will decrease if any production factor is decreased or the temperature is reduced. When using the re-burning method, since the amount of unburned hydrocarbons increases and they leave the furnace completely unburned, the amount of hydrogen atoms decreases in the environment. Also, the adiabatic temperature of the flame decreases. Consequently, less water is produced when the re-burning process is used. Figure 26 displays the mass fraction distribution of H₂O in the stoichiometric state and Case 4.

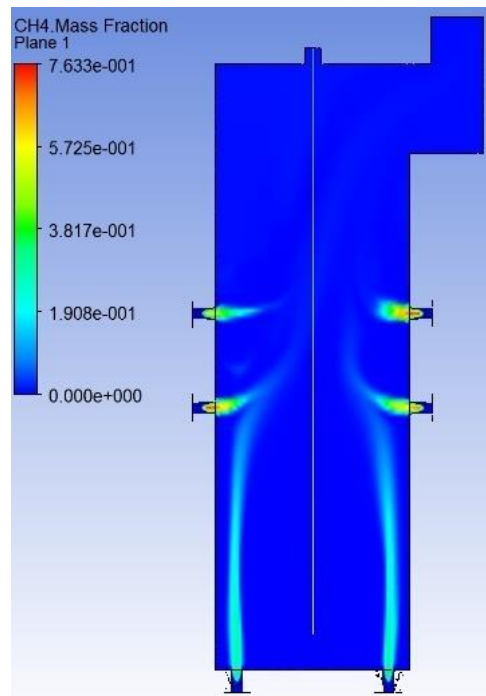


Figure 22. The distribution of CH4 in the stoichiometric state

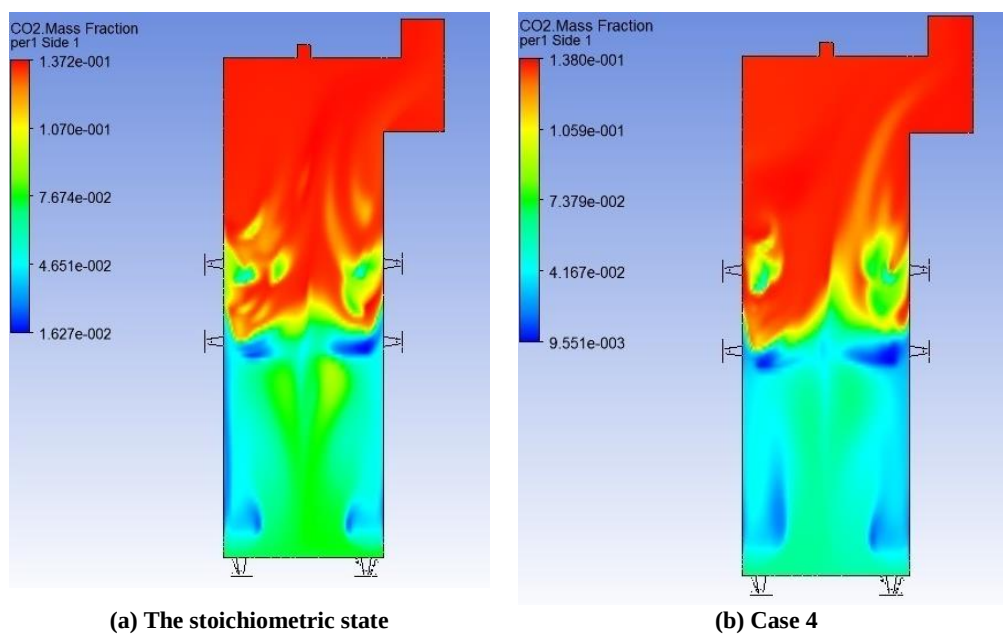


Figure 23. The distribution of CO2 inside the furnace

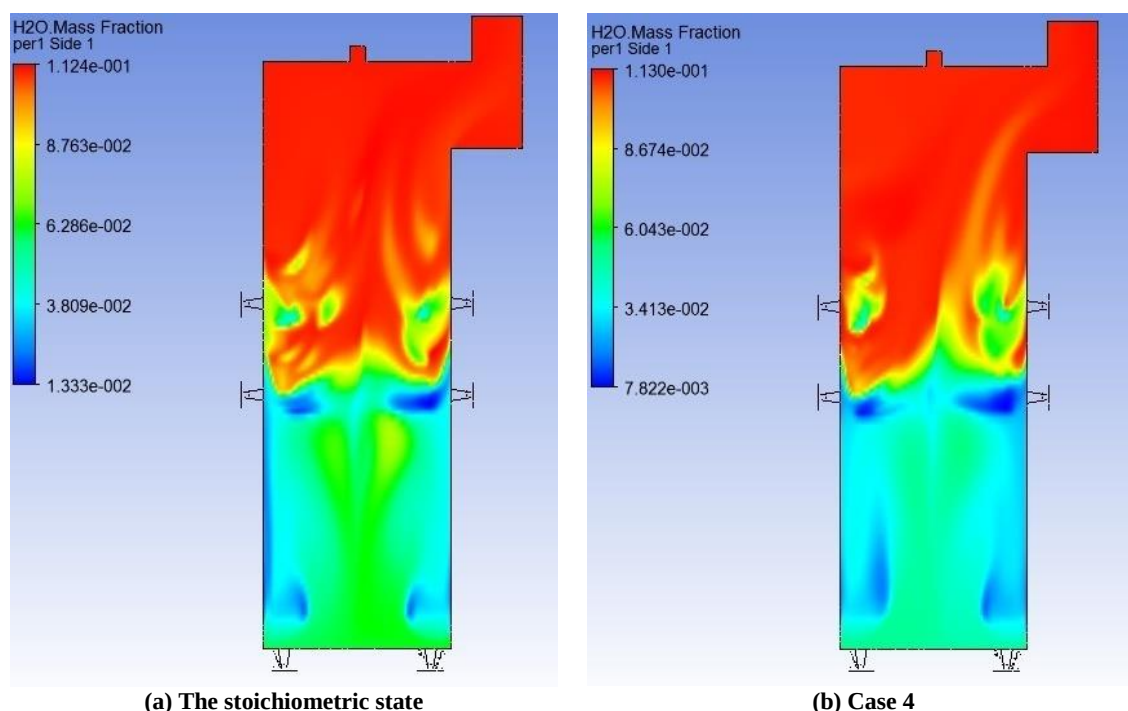


Figure 24. The distribution of H₂O inside the furnace

Here, we observe that the use of the re-burning method can be an effective step towards reducing NO_x emission. However, this needs extensive and expensive studies to study different cases of the balance ratios in the fuel-rich and fuel-poor regions and to optimize the air: fuel ratios of different burners by using neural network methods and genetic algorithms. Figure 25 shows the modeling of the flow field for Case 4. It is evident that the number of the return flow zones is similar to Ilam's furnace. The main difference is the shorter length of the two returning flow zones in the furnace centers and the creation of two other zones of returning flow in the vicinity of the wall-mounted burners.

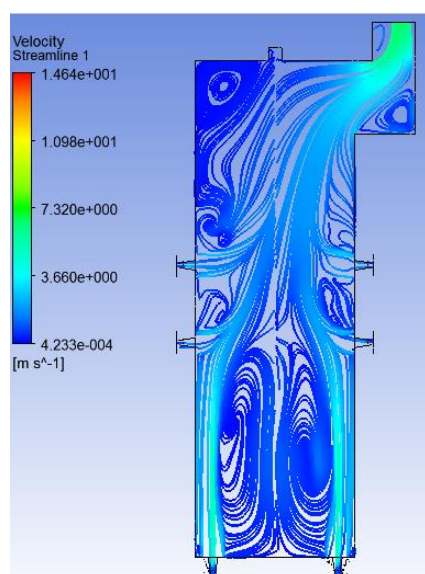


Figure 25. The flow field for Case 4

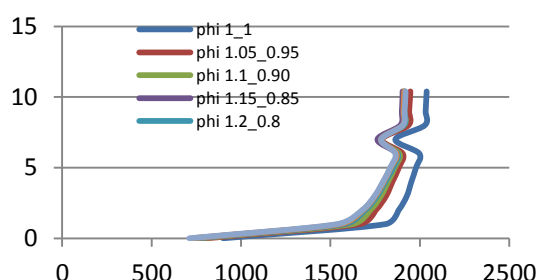


Figure 26. The mean temperature of the combustion gases inside the furnace at different cases

Eventually, Figure 26 shows the changes in the gas temperature in terms of height inside the furnace considering seven cases. It can be seen that the trend of temperature distribution along the furnace height is more uniform than that of Ilam's furnace (in which the burner is bottom-mounted). Also, as was already mentioned, the comparison of the seven cases shows that at the optimal state of NO_x reduction (Case 4), the temperature is lower and, consequently, the thermal power is lower than the stoichiometric case.

7 Conclusion

This research explored the results of modeling thermal cracking furnaces in two real-world cases. First, the thermal cracking reactor was modeled and after its results were verified by using real values, they were explored. Also, by changing the vision on furnace examination, the thermal cracking reactor of Maron was modeled and the efficiency of the re-burning method was examined to reduce NO_x emission of the combustion process. As was expected, the re-burning method is very effective in reducing NO_x emission and it helped realize the optimal target though it has some negative consequences. As the results revealed,

given the high capacities of the Olefin production, improving the production process or increasing product efficiency, even slightly, can enhance economic productivity considerably.

It is inferred from the results that the thermal flux is decreasing at a height of >3 m in a furnace, which can be offset by mounting low-power burners on the wall. As such, more uniform heat can be produced, and the process efficiency can be enhanced. Nonetheless, the installation of burners on walls is common in other furnaces.

Abbreviation and Nomenclature

abbreviation	description
CFD	Computational Fluid Dynamic
SFT	Swirl Flow Tube
EDC	eddy-dissipation-concept
CO	Carbon monoxide
Nox	Nitrogen oxides
RANS	Reynolds-Averaged Navier–Stokes
LES	large eddy simulation
DO	Discrete ordinate
τ_{ij}	stress tensor
Sm	source term
K_{eff}	Effective coefficient of conductivity
J'_j	Diffusion flux of the j' component
S_h	Heat of the chemical reaction

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