FOSSEE Semester Long Internship (Autumn) Report

On

Modelling and Simulation of Fired Heater and Venturi Scrubber on DWSIM

Submitted by

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<u>1.INTRODUCTION</u>

1.1 Background of process simulation

Process simulation is an essential tool in modern chemical engineering used to analyze, design, and optimize chemical processes through mathematical models and computer-based calculations. It allows engineers to represent real industrial processes in a virtual environment, enabling them to study system behavior under different operating conditions without the need for expensive or time-consuming physical experiments.

The concept of process simulation began developing in the **1950s and 1960s** with the advancement of digital computers. Early chemical process calculations were performed manually or using simple numerical methods. As computing power increased, specialized software was developed to simulate complex chemical processes involving mass transfer, heat transfer, thermodynamics, and chemical reactions. This led to the development of well-known commercial simulators such as Aspen Plus, HYSYS, and CHEMCAD.

Process simulation software uses fundamental engineering principles such as **material balance, energy balance, thermodynamic relationships, and transport phenomena** to model industrial equipment and processes. By solving these equations numerically, the simulator predicts important parameters such as temperature, pressure, flow rate, composition, and energy consumption throughout a process.I

Today, process simulation plays a critical role in **process design, equipment sizing, optimization, troubleshooting, and environmental analysis**. Engineers can evaluate multiple operating conditions, improve process efficiency, reduce energy consumption, and minimize environmental emissions before implementing the process in a real plant. This significantly reduces development cost and risk.

In addition to commercial software, open-source simulators such as DWSIM have become increasingly popular in academic research and education. These tools allow students and researchers to perform advanced process modelling and simulation without the high cost associated with proprietary software.

Overall, process simulation has become a fundamental component of chemical process engineering, enabling the development of safer, more efficient, and more sustainable industrial processes.

1.2 Importance of fired heater in industry

A **fired heater** is a critical piece of thermal equipment widely used in the **chemical, petrochemical, and refining industries** to heat process fluids to a required temperature using the combustion of fuels such as natural gas, fuel oil, or refinery gas. It transfers heat generated by burning fuel to process fluids flowing through tubes placed inside the heater.

Fired heaters are essential in many industrial operations because many chemical processes require **high temperatures to initiate or maintain reactions, vaporization, or separation processes**.

1. Process Heating

Fired heaters are primarily used to raise the temperature of process streams before they enter reactors, distillation columns, or other processing equipment. Heating the fluid improves reaction rates and ensures efficient separation or conversion of chemical compounds.

2. Petroleum Refining Operations

In petroleum refineries, fired heaters are used to heat crude oil and intermediate streams before they enter units such as atmospheric distillation columns, vacuum distillation units, and cracking units. Proper heating is necessary to vaporize hydrocarbons and enable efficient separation.

3. High Temperature Capability

Fired heaters can generate very high temperatures (often **400–1000°C**) which are difficult to achieve using conventional heat exchangers or steam heating. This makes them suitable for processes that require intense heat.

4. Energy Efficiency

Modern fired heaters are designed with **radiant and convection sections** that maximize heat recovery from combustion gases. This improves thermal efficiency and reduces fuel consumption, which is important for large-scale industrial operations.

5. Flexibility in Fuel Usage

Fired heaters can operate using different fuels such as natural gas, refinery gas, fuel oil, or process off-gases. This flexibility allows industries to utilize by-products as fuel, improving overall plant economics.

1.3 Importance of Venturi Scrubber in Pollution control

Efficient Removal of Particulate Matter

Venturi scrubbers are highly effective in removing **fine particles such as dust, fly ash, and metal oxides** from industrial exhaust gases. The gas accelerates through the narrow **venturi throat**, where liquid is injected and forms fine droplets. These droplets collide with particles in the gas stream, capturing them and removing them from the gas.

2. Control of Hazardous Air Pollutants

Many industries release harmful pollutants such as sulfur compounds, acidic gases, and toxic particulates. Venturi scrubbers help reduce these emissions, preventing environmental contamination and protecting public health.

3. Removal of Very Fine Particles

Unlike many conventional pollution control devices, venturi scrubbers can remove **very small particles (even below 1 µm)** due to the strong turbulence and high relative velocity between gas and liquid droplets.

4. Application in Flue Gas Cleaning

Venturi scrubbers are widely used for **flue gas cleaning** in industries such as:

Thermal power plants (removal of fly ash)

Steel and metallurgical industries

Chemical processing plants

Fertilizer industries

They help industries comply with **environmental emission regulations**.

5. Simultaneous Gas and Particle Removal

Venturi scrubbers can remove both **particulate pollutants and some gaseous contaminants** simultaneously, making them versatile pollution control devices.

6. Industrial Reliability and Simple Operation

These scrubbers have a relatively **simple design with no moving parts**, making them reliable and suitable for handling high-temperature and high-dust gas streams.

7. Role in Process Simulation and Design

In process simulation tools such as DWSIM, venturi scrubbers can be modeled to analyze parameters such as:

- Gas velocity in the venturi throat
- Pressure drop across the scrubber
- Droplet size and relative velocity
- Particle collection efficiency

1.4 Objective

The objective of this study is to develop and analyze models of a fired heater and a venturi scrubber using the process simulation software DWSIM. The study aims to understand the working principles and operating behavior of these important industrial units through simulation. By modelling these systems, the performance parameters such as temperature, heat transfer, gas velocity, and pressure drop can be evaluated under different operating conditions. The work also helps in gaining practical knowledge of process simulation techniques and understanding how simulation tools can be used to study and optimize industrial processes.

2.LITERATURE REVIEW

2.1 Modeling and optimization of process fired heaters

- Reserachers-Mojtaba Haratiana , Majid Amidpourb,c,⁎ , Aliasghar Hamidi

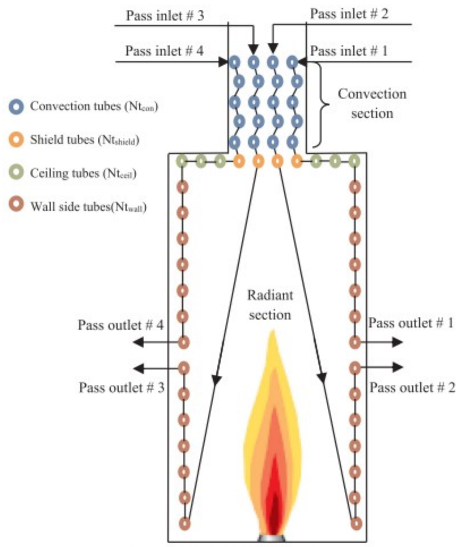


Fig. 3. A four-pass fired heat layout.

Fired heaters are widely used in petroleum refineries and petrochemical industries for heating process fluids such as crude oil and hydrocarbon mixtures. In these systems, the process fluid flows through tubes and is heated by hot gases generated from fuel combustion. Due to their high energy consumption and operational cost, efficient design and optimization of fired heaters is essential for improving thermal efficiency and reducing operating expenses. The research paper titled **"Modeling and Optimization of Process Fired Heaters"** presents a mathematical modeling and optimization approach to improve the design and economic performance of fired heaters.

The main objective of the study is to develop a mathematical model capable of describing the thermal behavior, geometric design, and operational characteristics of fired heaters. The proposed model considers different sections of a typical fired heater including the **radiant section, convection section, and stack**. The process fluid first passes through the convection section where it is heated by hot flue gases through convective heat transfer. After that, the fluid enters the radiant section where the majority of heat transfer occurs through thermal radiation from the combustion gases. Finally, the flue gases exit through the stack after transferring most of their heat energy.

The modeling of the fired heater is based on fundamental principles such as **mass balance, energy balance, and heat transfer correlations**. The study uses the **Lobo–**

Evans method, which is a widely accepted engineering approach for analyzing heat transfer in fired heaters. The model includes equations for calculating radiant heat transfer, convection heat transfer, tube heat transfer area, furnace dimensions, pressure drop, and fuel consumption. Several important design parameters such as tube diameter, tube length, furnace width, number of passes, radiant heat flux, furnace efficiency, and excess air are considered in the model.

In addition to thermal analysis, the model also considers **hydraulic design and pressure drop calculations**. Pressure drop inside the tubes is an important parameter because excessive pressure losses can increase pumping power requirements and operating cost. Therefore, the design must ensure that the pressure drop remains within acceptable limits while still achieving efficient heat transfer.

To determine the optimal design parameters, the researchers applied **Genetic Algorithms (GA)** as an optimization technique. Genetic algorithms are evolutionary optimization methods inspired by the process of natural selection. They are particularly useful for solving complex nonlinear optimization problems involving multiple variables and constraints. In this study, the genetic algorithm was implemented using MATLAB to search for the best combination of design variables that minimizes the overall cost of the fired heater.

The objective function used for optimization is the **Total Annual Cost (TAC)**. This cost includes both **capital cost** and **operating cost**. Capital cost mainly depends on the size of the heater, heat transfer surface area, and furnace structure. Operating cost is primarily determined by fuel consumption required to maintain the desired heating duty. By minimizing TAC, the model aims to achieve the most economical heater design.

The researchers investigated two optimization scenarios. In the first scenario, several design variables such as number of passes, furnace efficiency, radiant heat flux, firebox width, tube length, and gas velocity in the stack were optimized while tube diameter and excess air were kept constant. In the second scenario, additional variables including **tube diameter and excess air** were also included in the optimization process. The results showed that increasing the number of decision variables provides greater flexibility in the design and can potentially reduce the overall cost of the system.

However, the results also indicated that minimizing only the total annual cost may lead to unrealistic designs in some cases. For example, reducing the tube diameter too much can significantly increase the pressure drop in the tubes, which exceeds the allowable operating limits. To address this issue, the researchers introduced a modified objective function that includes the **pumping power cost** required to overcome the pressure drop in the system. This new objective function is referred to as the **Modified Total Annual Cost (MTAC)**.

By incorporating the pumping cost into the operating cost, the optimization process was able to produce designs that are both economically efficient and technically feasible. The results demonstrated that the optimized design obtained using the modified objective function reduced the total annual cost by approximately **2.48% compared to the original design** while maintaining acceptable pressure drop and operational conditions.

The study also validated the developed mathematical model by comparing the results with previously published literature. The comparison showed good agreement between the predicted values and the reference data, confirming the reliability and accuracy of the model.

In conclusion, the research demonstrates that combining **mathematical modeling with genetic algorithm optimization** is an effective method for improving the design of process fired heaters. The proposed approach allows engineers to analyze the influence of different design parameters, reduce fuel consumption, and minimize the overall cost of the heating system. Furthermore, the inclusion of pumping power cost in the optimization process ensures that the final design remains practical and operationally safe. This methodology can be applied to the design and optimization of industrial fired heaters in refineries and petrochemical plants to enhance energy efficiency and economic performance.

2.2Dust Particle Removal Efficiency of a Venturi Scrubber:

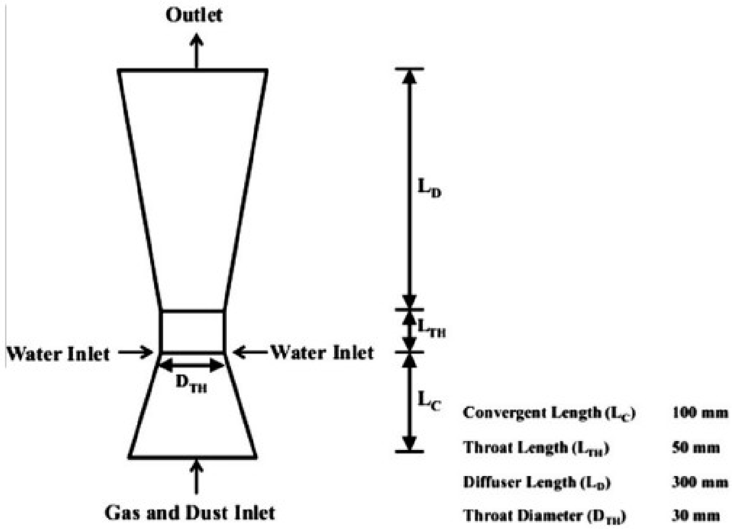


Fig. 2. Schemtaic diagram of venturi scrubber.

Venturi scrubbers are widely used air pollution control devices designed to remove particulate matter and gaseous contaminants from industrial gas streams. They are particularly effective for capturing fine particles due to the high relative velocity between gas and liquid droplets inside the scrubber. The research paper titled **"Dust Particle Removal Efficiency of a Venturi Scrubber"** investigates the removal efficiency of dust particles using a self-priming venturi scrubber and develops a mathematical model to explain the particle capture mechanism.

The main objective of the study is to experimentally analyze how different operating parameters such as gas velocity, liquid flow rate, and dust concentration influence the performance of a venturi scrubber. Venturi scrubbers operate by injecting liquid into a high-velocity gas stream. The liquid breaks into very fine droplets, which collide with and capture dust particles due to inertial impaction, interception, and diffusion mechanisms. The captured particles are then removed from the gas stream along with the liquid droplets.

The study highlights that venturi scrubbers are commonly used in industries because they offer several advantages. These include simple design, compact size, absence of moving parts, and the ability to handle high-temperature and corrosive gases. Additionally, venturi scrubbers can remove both particulate matter and certain gaseous pollutants simultaneously, making them suitable for pollution control applications in power plants, chemical industries, and environmental protection systems.

To evaluate the performance of the scrubber, an experimental setup was developed consisting of an air compressor, air tank, venturi scrubber, water tank, dust injection system, and sampling ports for measuring dust concentration. The schematic diagram of the experimental setup is shown on **page 3 of the paper**, where gas mixed with dust particles enters the venturi scrubber and water is injected to form droplets that capture the particles. The inlet and outlet dust concentrations were measured using filtration techniques to determine the overall removal efficiency.

The venturi scrubber used in the experiment had specific geometric parameters including a convergent section length of **100 mm**, throat length of **50 mm**, diffuser length of **300 mm**, and throat diameter of **30 mm**, as shown in the schematic diagram on **page 3**. The scrubber was operated at different throat gas velocities of **130 m/s, 165 m/s, and 200 m/s** and liquid flow rates ranging from **0.3 m^3/h to 1 m^3/h**. Dust concentration levels were maintained between **0.1 g/m^3 and 1 g/m^3** using titanium dioxide particles with a diameter of approximately **1 µm**.

In addition to experimental work, the researchers developed a mathematical model to describe the particle removal process inside the venturi scrubber. The model is based on several simplifying assumptions such as uniform droplet size, co-flow of gas and droplets, absence of droplet coalescence, and uniform droplet distribution. The model primarily considers **inertial impaction** as the dominant particle capture mechanism, particularly for particles with sizes around 1 µm. The motion of droplets and particles is analyzed using equations based on drag force, relative velocity between gas and droplets, and droplet size correlations.

The study also introduces the concept of **single droplet collection efficiency**, which describes the ability of a single liquid droplet to capture particles. This efficiency depends on factors such as droplet diameter, particle size, fluid velocity, and Stokes number. The overall dust removal efficiency of the scrubber is calculated using a mathematical expression that relates inlet and outlet dust concentrations with the interaction between particles and droplets inside the venturi throat.

Experimental results show that the **dust removal efficiency increases with increasing throat gas velocity and liquid flow rate**. Higher gas velocities lead to stronger turbulence and higher relative velocity between particles and droplets, which enhances the collision probability. Similarly, increasing the liquid flow rate produces a larger number of droplets, increasing the surface area available for particle capture. These effects significantly improve the overall removal efficiency of the venturi scrubber.

The results also indicate that dust concentration has a smaller influence on removal efficiency compared to gas velocity and liquid flow rate. At higher throat velocities, the droplets become smaller due to atomization, increasing their surface area and improving particle capture efficiency. According to the experimental findings, the

maximum dust removal efficiency achieved in the study was approximately 99.5% at a throat gas velocity of 200 m/s.

To verify the validity of the mathematical model, the researchers compared the predicted removal efficiency with the experimental data. The comparison graph presented on **page 5 of the paper** shows good agreement between calculated and measured efficiencies. This confirms that the proposed model successfully explains the particle capture mechanism inside the venturi scrubber.

In conclusion, the study demonstrates that venturi scrubbers are highly efficient devices for removing fine dust particles from gas streams. The performance of the scrubber is strongly influenced by operating parameters such as throat gas velocity and liquid flow rate. Increasing these parameters enhances particle–droplet interactions and improves removal efficiency. The developed mathematical model based on inertial impaction provides a reliable method for predicting the performance of venturi scrubbers and can be used for design and optimization of industrial gas cleaning systems

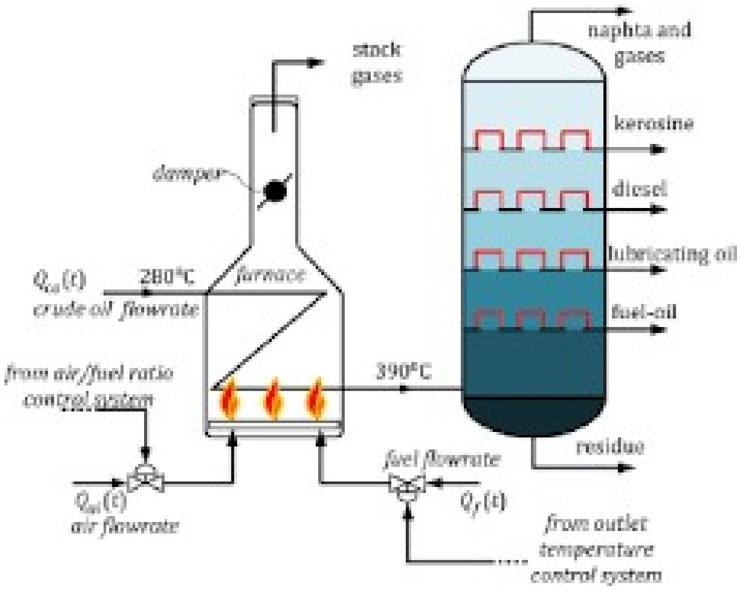
3.MODELLING AND SIMULATION OF FIRED HEATER

3.1 Introduction to Fired Heaters:

A fired heater is an important industrial heating device widely used in petroleum refineries, petrochemical plants, and chemical processing industries. It is designed to heat process fluids such as crude oil, hydrocarbons, or chemical feedstocks by using the heat generated from fuel combustion. In a fired heater, fuel such as natural gas, fuel oil, or refinery gas is burned inside a furnace, producing high-temperature flue gases. These hot gases transfer heat to the process fluid flowing through tubes placed inside the heater.

3.2 Industrial Applications of Fired Heaters:

Fired heaters are widely used in many industrial processes where large amounts of heat are required to raise the temperature of fluids or initiate chemical reactions. These heaters are essential in petroleum refining, petrochemical production, chemical manufacturing, and power generation industries. Their ability to deliver high heat duty and operate at elevated temperatures makes them a critical component of many industrial processing units.
One of the most important applications of fired heaters is in **petroleum refineries**, particularly in **crude oil distillation units (CDU)**. In this process, crude oil must be heated to high temperatures before entering the distillation column. The fired heater raises the temperature of crude oil to around 350–400°C so that it can be separated into different fractions such as gasoline, kerosene, diesel, and heavy oils inside the distillation tower.



3.3 Working Principle:

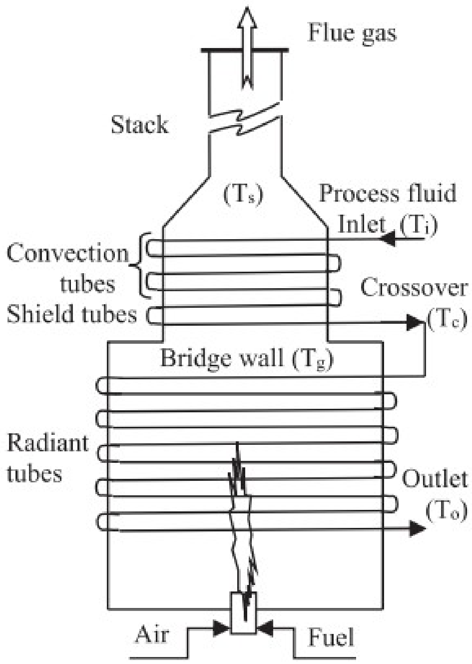


Fig. 1. Flow sketch of a cabin type fired heater.

A typical fired heater consists of **three main sections: the radiant section, the convection section, and the stack**. Each section plays a specific role in the heating process.

1. Radiant Section

The radiant section is the **primary heating zone** of the fired heater where most of the heat transfer occurs. In this section, burners produce flames and hot combustion gases that generate very high temperatures. The process fluid flows through tubes arranged along the walls or floor of the furnace. Heat transfer in this region occurs mainly through **thermal radiation from the flame and hot flue gases to the tube surfaces**.

According to the research model, nearly **90% of heat transfer in this zone occurs by radiation**, while the remaining heat is transferred by convection. The radiant section is designed to provide intense heating so that the fluid reaches the required high temperature before leaving the furnace.

2. Convection Section

The convection section is located **above the radiant section** and is used to recover additional heat from the flue gases before they leave the heater. After transferring heat in the radiant zone, the combustion gases still contain significant thermal energy. In the convection section, these gases flow over banks of tubes carrying the process fluid. Heat transfer here occurs mainly through **convective heat transfer** between the hot gases and the tube surfaces.

The convection section improves the overall thermal efficiency of the fired heater by utilizing waste heat from the flue gases. The fluid entering this section is preheated before it reaches the radiant section, which reduces the amount of fuel required for heating.

3. Stack (Chimney)

The stack, also known as the **chimney**, is the final section of the fired heater. Its main function is to **discharge flue gases safely into the atmosphere** and maintain proper draft inside the furnace. The stack creates a slight negative pressure that allows fresh air to enter the burners and ensures continuous combustion.

In addition to removing combustion gases, the stack also helps control furnace pressure and stabilize the flow of flue gases through the heater. The temperature of gases leaving the stack is typically lower because most of the heat has already been transferred to the process fluid in the radiant and convection sections.

3.4 Mathematical Model and Governing Equations:

The heat balance for a fired heater is expressed by Eq. (A1).

$$Q_f = Q_{rad} + Q_{con} + Q_{loss} + Q_s \tag{A1}$$

where Q_{loss} is the heat loss rate through the furnace walls which is about 2–3% of the heat generated by the fuel (Q_f) and Q_s is the heat content of the gas leaving the convection section [22]. Here, the percent of heat loss to the surrounding is assumed 2.5%. Q_{rad} and Q_{con} are the heat transfer rates to the process fluid in radiant and convection zones, respectively.

The heat duty of a fired heater (Q_A) can be computed as:

$$Q_A = M_{pf}(h_o - h_i) = Q_{rad} + Q_{con} \tag{A2}$$

where h_i and h_o are the enthalpies of inlet and outlet process fluid, respectively.

The radiant duty fraction (Rdf) is defined as the ratio of radiant heating (Q_{rad}) to the heat absorbed (Q_A). The radiant duty fraction can be initially assumed as 75% of the total heat duty [22].

The heat generated by the combustion process (Q_f) is calculated as:

$$Q_f = M_f * LHV = \frac{Q_A}{\eta_F} \tag{A3}$$

where M_f, LHV and h_F are the rate of fuel consumption, the lower calorific value and the furnace efficiency, respectively.

For the given tube diameter (D_i) and flow rate of the process fluid (M_{pf}), the number of required passes is represented by Eq. (A4).

$$N_{pass} = \frac{M_{pf}}{\rho A_c V_{pf}} \tag{A4}$$

where A_c is the cross section area of the tube, ρ and V_{pf} are the density and velocity of the process fluid, respectively.

Heat transfer in the radiant section of a fired heater is given by Eq. (A5) [22],

$$\frac{Q_{rad}}{\alpha A_{cp} F} = 1730\left[\left(\frac{T_g + 460}{1000}\right)^4 - \left(\frac{T_t + 460}{1000}\right)^4\right] + 7(T_g\_T_t) \tag{A5}$$

where T_g and T_t are the effective gas temperature and the average tube skin temperature in the radiant zone, respectively. In addition, α, A_{cp}, and F are defined as the tube surface absorptivity, the cold plan area and the exchange factor, respectively.

The required number of tubes in the radiant zone (Nt_{rad}) is computed as follows:

$$Nt_{rad} = \frac{Q_{rad}}{Flux * \pi D_o L} \tag{A6}$$

where D_o is the outer diameter of the tube and L is the exposed length of the tubes in the radiant zone which is calculated as:

$$L = L_a - K_a \tag{A7}$$

where K_a refers to the unexposed length of the tube. In this model, L_a is the tube length which is considered as input data between 12 and 16 m. Usually, the exposed length of the tube (L) is 0.45 m shorter than the tube length [22,23].

The total number of tubes in the radiant section is obtained as:

$$Nt_{rad} = Nt_{wall} + Nt_{ceil} + Nt_{shield} \tag{A8}$$

The following constraints are presented to estimate the dimensions of the radiant zone [21]:

$$W_c = (Nt_{shield} - 1) * cc + kk_1 \tag{A9}$$

$$W - W_c \geq (Nt_{ceil} - 1) * cc + kk_2 \tag{A10}$$

$$H = \left(\frac{Nt_{wall}}{2} - 1\right) * cc + kk_3 \tag{A11}$$

$$3.5 < \frac{L * W * H}{\pi D_o L Nt_{rad}} < 4.5 \tag{A12}$$

$$1 \leq \frac{H}{W} \leq 1.5 \tag{A13}$$

$$1.8 \leq \frac{L}{W} \leq 3 \tag{A14}$$

$$\frac{Q_{gc}}{Q_f} = \left(\frac{T_g}{1000} - 0.1\right)\left[X_1 + X_2\left(\frac{T_g}{1000} - 0.1\right)\right]$$
$$X_1 = 0.22048 - 0.35027ex + 0.92344ex^2$$
$$X_2 = 0.016086 + 0.29393ex - 0.48139ex^2 \tag{A15}$$

The physical properties of process fluid, based on the temperature of fluid (T_{pf}) can be estimated as follows [7,31]:

$$\text{Specific Gravity:} \quad SG = SG_{15} - (5.93 * 10^{-4}) * (T_{pf} - 15) \tag{A16}$$

$$\text{Heat capacity:} \quad C_p = (2 * 10^{-3} * T_{pf} - 1.429) * SG + 2.67 * 10^{-3} * T_{pf} + 3.049 \tag{A17}$$

$$\text{Thermal conductivity:} \quad k = 0.49744 - 29.4604 * 10^{-5} * T_{pf} \tag{A18}$$

$$\text{Viscosity:} \quad \ln(\mu) = -0.2207 * \ln^2(T_{pf}) + 0.5052 * \ln(T_{pf}) - 11.8201 \tag{A19}$$

where SG_{15} is the specific gravity of crude oil at 15 (°C).

Appendix B. Convection section

Heat transfer in the convection section is given by,

$$Q_{con} = U_c \cdot A_{con} \cdot LMTD \tag{B1}$$

The logarithmic mean temperature difference is represented as:

$$LMTD = \frac{(T_g - T_c) - (T_s - T_i)}{\ln\left(\frac{T_g - T_c}{T_s - T_i}\right)} \tag{B2}$$

The cross-over temperature of process fluid from convection to radiant section (T_c) can be determined from the energy balance for the process fluid in the radiant zone. The stack inlet temperature (T_s) can also be computed considering Eqs. (A1) and (A15).

The overall heat transfer coefficient in the convection section depends on the total apparent gas film coefficient outside the tubes (h_{co}) and the convection heat transfer coefficient inside the tubes (h_{ci}).

$$U_c = \frac{h_{co} \cdot h_{ci}}{h_{co} + h_{ci}} \tag{B3}$$

The total apparent gas film coefficient is calculated as:

$$h_{co} = (1 + f)(h_{cc} + h_{cr}) \tag{B4}$$

The following equations compute the individual heat transfer coefficients (h_{cc}, h_{cr}) that correspond to the convective gas film and the flue gas radiation coefficients, respectively [7,21].

$$h_{cc} = 0.018 c_{p_{fluegas}} \left(\frac{G_{max}^{2/3} \cdot T_{gf}^{0.3}}{D_o^{1/3}} \right) \tag{B5}$$

$$T_{gf} = 0.5(T_i + T_c) + 0.5LMTD \tag{B6}$$

$$h_{cr} = 0.092 T_{gc} - 34 \tag{B7}$$

$$T_{gc} = 0.5(T_i + T_c) + LMTD \tag{B8}$$

where $c_{p_{fluegas}}$ is the average specific heat capacity of flue gas, T_{gf} and T_{gc} are the average gas film temperature and the average gas temperature in the convection zone and G_{max} is the maximum flue gas rate at the minimum cross section in the convection zone.

In Eq. (B4) f is a coefficient factor based on re-radiation from the refractory walls of the convection section. This factor usually ranges from 6 to 15% of the sum convective gas film and flue gas radiation coefficients [7]. A value of 10% is considered as a typical average.

For turbulent flow, 10000 $< Re <$ 120,000 and $L/D_o > 60$, the tube convection heat transfer coefficient, is represented by [7]:

$$h_{ci} = 0.023 \left(\frac{K}{D_i} \right) Pr^{1/3} Re_{Di}^{0.8} \left(\frac{\mu}{\mu_w} \right)^{0.14} \tag{B9}$$

where K, Pr and μ refer to the thermal conductivity, Prantdtl number and viscosity of the process fluid, respectively. They are computed at the average temperature of the process fluid and μ_w is computed at the tube-wall temperature. The required number of tubes (Nt_{con}) and rows (Row_{con}) in the convection zone are presented as follows:

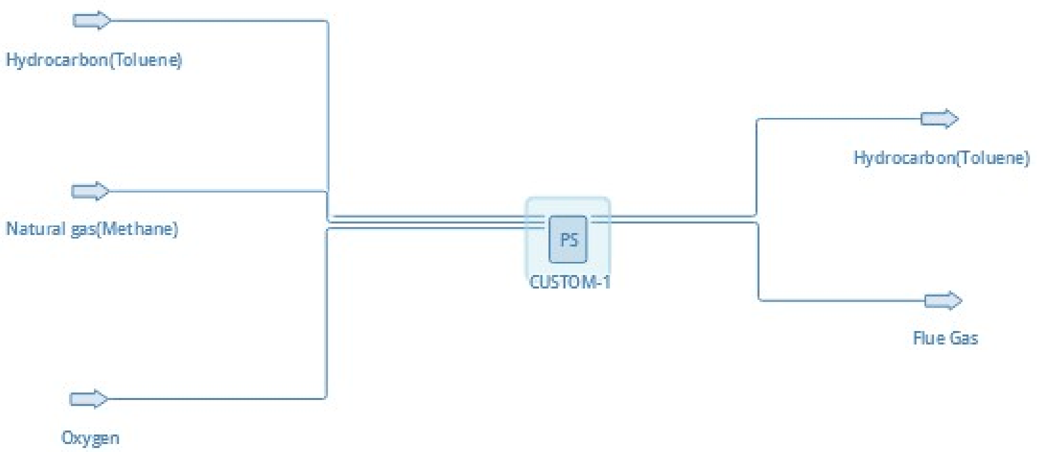
$$Nt_{con} = \frac{Q_{con}}{U_c * LMTD * \pi D_o L} \tag{B10}$$

$$Row_{con} = \frac{Nt_{con}}{Nt_{shield}} \tag{B11}$$

The tube side pressure drop for single-phase process fluid can be estimated using the equation:

$$\Delta P_i = \frac{0.00517 f v G^2}{D_i} L_e \tag{B12}$$

3.5 Simulation Procedure:



The modelling and simulation of the fired heater were carried out in **DWSIM using IronPython scripting** to represent the heat transfer and flow behaviour in different sections of the heater. The simulation integrates thermodynamic properties of process streams with mathematical correlations describing heat transfer, fluid flow, and draft calculations.

Initially, all the required **design parameters and operating conditions** such as gas temperatures, outlet temperature, ambient temperature, tube dimensions, stack height, flue gas velocity, and heater efficiency were defined as input variables. Additional constants such as friction factor, lower heating value of fuel, radiation coefficients, and geometrical ratios were also specified to represent the furnace configuration.

The simulation obtains **thermophysical properties of the feed streams directly from the DWSIM flowsheet**. Three inlet streams were considered: hydrocarbon feed, methane fuel, and oxygen. Using built-in DWSIM functions, properties such as heat capacity, thermal conductivity, density, viscosity, pressure, temperature, and flow rate were extracted from each stream. These values are required to evaluate transport phenomena and energy balances within the heater.

The **convection section of the fired heater** was modelled first. The gas velocity inside the tubes was calculated using the mass flow rate, density, and tube diameter. The **log mean temperature difference (LMTD)** between the flue gas and process fluid was determined to evaluate the driving force for heat transfer. Using empirical correlations, the **external convection heat transfer coefficient** was calculated considering both convective and radiative components of flue gas heat transfer. The internal heat transfer coefficient was then determined using dimensionless correlations involving the Reynolds number and Prandtl number. From these coefficients, the **overall heat transfer coefficient** was evaluated, which allowed calculation of the required heat transfer area and number of convection tubes.

Next, the **radiant section** was analysed. The heat duty required to raise the feed temperature to the desired outlet temperature was calculated using the energy balance equation. A portion of this heat duty was assumed to be transferred in the radiant zone. The required radiant surface area was estimated using radiation heat transfer correlations involving furnace gas temperature and tube skin temperature. From this surface area, the **number of radiant tubes** required for the heater was determined. Furnace geometry parameters such as chamber width, height, and the number of shield tubes were also estimated based on specified design ratios.

Finally, the **stack and draft calculations** were performed. The natural draft generated by the stack was evaluated using the difference in density between hot flue gases and ambient air. Pressure losses occurring in the convection bank, stack, and radiant section were calculated using empirical pressure drop correlations. These values were compared with the available draft to determine whether the furnace operates under sufficient natural draft conditions.

After completing all calculations, the program writes the calculated results such as **number of radiant tubes, number of convection tubes, and total pressure drop** to the DWSIM message window. The outlet stream temperatures were then updated in the flowsheet to represent the heating effect of the fired heater.

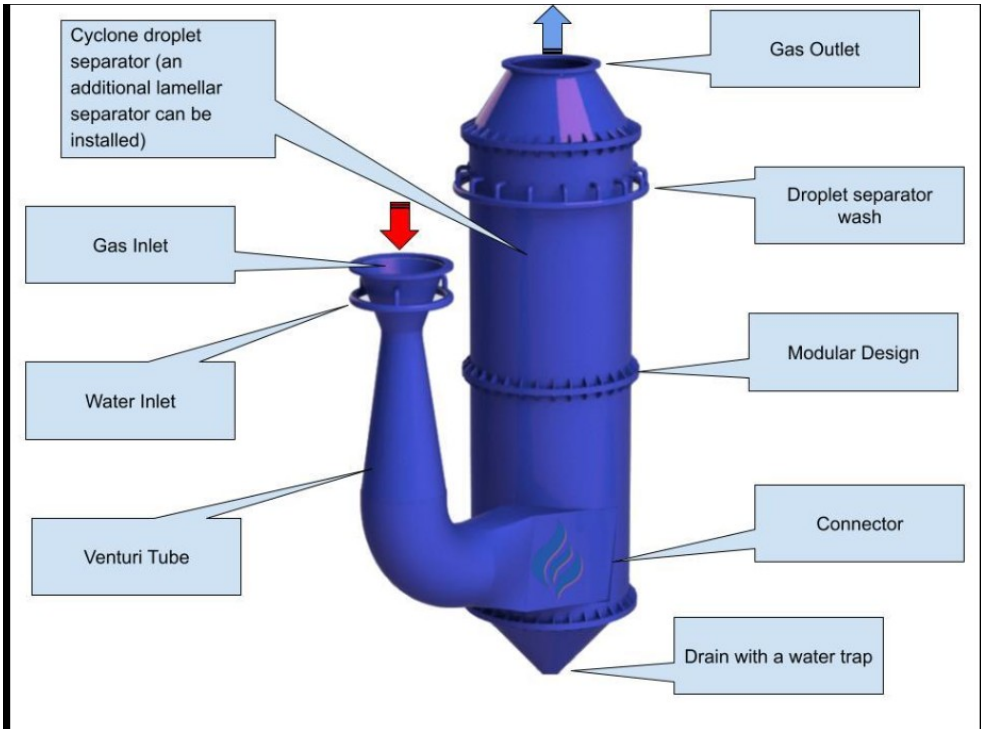
Thus, the IronPython script integrates **heat transfer correlations, furnace design equations, and thermodynamic property calculations** to simulate the performance of the fired heater within the DWSIM environment.

3.6 Results and Discussion:(DWSIM Results)

3	3/12/2026 12:00:06 AM	Message	The flowsheet was calculated successfully. [2.212s]
2	3/12/2026 12:00:06 AM	Message	Pressure drop in fired heater= 100.16838369763455Pa
1	3/12/2026 12:00:06 AM	Message	Number of convection tubes= 964.25542406471243
0	3/12/2026 12:00:06 AM	Message	Number of radiant tubes= 1166.6667245520728

4.Modelling and Simulation of Venturi Scrubber:

4.1 Introduction to Venturi Scrubbers:



A **venturi scrubber** is a highly efficient air pollution control device used to remove **particulate matter and gaseous pollutants from industrial gas streams**. It is widely applied in industries where flue gases contain fine particles, toxic gases, or aerosols that must be removed before releasing the gas into the atmosphere. The device operates based on the **principle of high-velocity gas-liquid contact**, which enhances mass transfer and particle capture.

The scrubber consists of three main sections: a **converging section, throat, and diverging section**. Contaminated gas enters the converging section where its velocity increases due to a reduction in cross-sectional area. At the **throat region**, the gas reaches very high velocities, typically between **60–120 m/s**, creating strong turbulence. A scrubbing liquid, usually water, is introduced into this region. The high gas velocity atomizes the liquid into very fine droplets, producing a large surface area for interaction between the gas and liquid phases.

As the gas stream passes through the throat, **dust particles and aerosols collide with the liquid droplets** due to inertial impaction and diffusion mechanisms. These particles become captured by the droplets, forming a liquid–solid mixture. The gas then enters the **diverging section**, where the velocity decreases and pressure partially recovers. The droplet–particle mixture is subsequently separated from the cleaned gas in a downstream separator such as a **cyclone or demister**.

Venturi scrubbers are particularly effective for removing **fine particulate matter smaller than 2.5 µm**, which are difficult to capture using conventional collectors. Because of the intense mixing and high turbulence, they can also remove certain **gaseous pollutants such as sulfur dioxide, hydrogen chloride, and ammonia** when an appropriate absorbing liquid is used.

4.2 **Industrial Applications:**

- **Thermal Power Plants:** Venturi scrubbers are used to remove **fly ash and fine particulate matter** from flue gases generated during coal combustion before the gases are released into the atmosphere.
- **Cement Industry:** They control **cement dust and silica particles** produced during clinker production, grinding, and material handling processes.
- · **Steel and Metallurgical Industries:** Venturi scrubbers remove **metal oxides, slag particles, and other aerosols** generated during blast furnace operations, metal smelting, and refining.
- · **Chemical and Petrochemical Industries:** They are used to remove **acid mists, sulfur compounds, and other hazardous gases** from exhaust streams of chemical processing units.
- **Fertilizer Industry:** Venturi scrubbers help in capturing **ammonia fumes, dust particles, and other gaseous pollutants** produced during fertilizer manufacturing.
- **Pharmaceutical Industry:** They are used to remove **fine powder particles and toxic vapors** generated during drug manufacturing processes.
- **Mining and Mineral Processing:** Venturi scrubbers control **dust emissions from crushing, grinding, and ore processing operations**.
- **Waste Incineration Plants:** They help remove **toxic particulates, ash, and acidic gases** from combustion gases before discharge.

4.3 Working Principle:

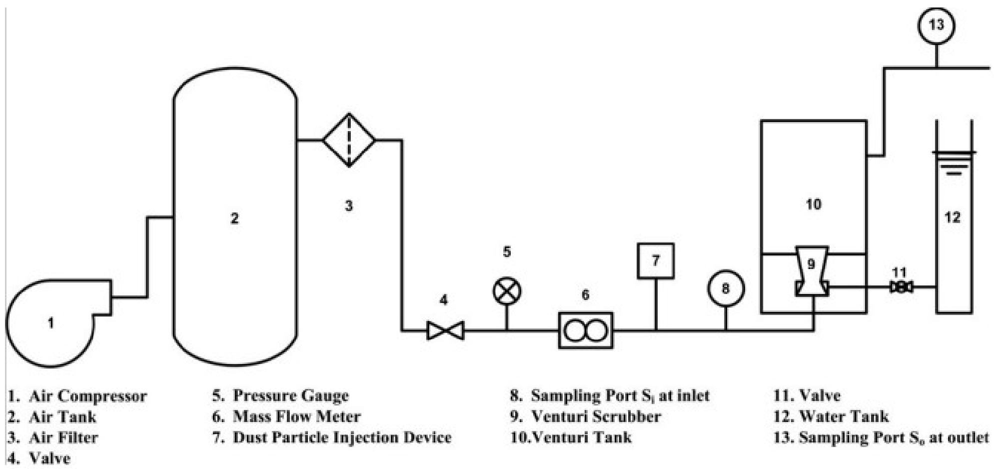


Fig. 1. Experimental setup for dust removal efficiency of venturi scrubber.

A venturi scrubber operates on the principle of **high velocity gas–liquid contact to remove particulate matter and pollutants from gas streams**. The device uses the **venturi effect**, where the velocity of a gas increases as it passes through a constricted section, creating intense turbulence and strong interaction between the gas and scrubbing liquid.

The contaminated gas first enters the **converging section** of the scrubber. In this section, the cross-sectional area decreases, causing the gas velocity to increase. This increase in velocity prepares the gas stream for effective mixing with the scrubbing liquid.

The gas then passes through the **throat section**, which is the narrowest part of the venturi scrubber. At this point, the gas velocity becomes very high, typically ranging from **60–120 m/s**. The scrubbing liquid, usually water, is introduced either at the entrance of the throat or directly into the throat. Due to the high gas velocity, the liquid breaks into **very fine droplets**, producing a large surface area for contact between the gas and liquid phases.

As the gas flows through the throat, **dust particles and aerosols collide with the liquid droplets** due to inertial impaction, interception, and diffusion mechanisms. These particles attach to the droplets and become captured by the liquid phase.

After the throat, the gas enters the **diverging section**, where the cross-sectional area increases and the gas velocity decreases. During this stage, some pressure recovery occurs and the droplet–particle mixture moves toward a **separator or demister**, where the liquid containing the captured particles is removed from the gas stream.

Finally, the **cleaned gas leaves the scrubber**, while the contaminated liquid is collected and treated or recycled. Through this mechanism, venturi scrubbers can effectively remove **fine particulate matter and certain gaseous pollutants** from industrial exhaust gases.

4.4 Mathematical Model and Governing Equations:

$$D_d = \frac{0.585}{v_r}\sqrt{\frac{\sigma}{\rho_l}} + 1.683 \times 10^{-3}\left(\frac{\mu_l}{\sqrt{\sigma\rho_l}}\right)^{0.45}\left(\frac{1000Q_l}{Q_g}\right)^{1.5} \tag{4}$$

Velocity of droplet calculated from the equation of motion of droplet (Boll, 1973),

$$\frac{dv_d}{dt} = \frac{3\mu_g C_D}{4\rho_d D_d}(v_g - v_d)^2 \tag{5}$$

Since the flow is against the gravity, therefore,

$$\frac{dv_d}{dt} = \frac{3\mu_g C_D}{4\rho_d D_d}(v_g - v_d)^2 - g \tag{6}$$

$$v_d = v_{d_i} + \int_0^t \frac{dv_d}{dt}dt \tag{7}$$

$$C_d = 0.22 + \frac{24}{Re}(1 + 0.15\mathrm{Re}^{0.6}) \quad (8)$$

3.3. Single droplet collection efficiency

The target efficiency of a single droplet η is calculated from inertial impaction mechanism which is a function of Stokes number. This phenomenon is more dominant for particle size of 1 μm (Lim et al., 2006). The impaction of single droplet efficiency is defined as (Calvert, 1970),

$$\eta = \left(\frac{\psi}{\psi + 0.7}\right)^2 \quad (9)$$

where ψ is expressed as (Pak and Chang, 2006),

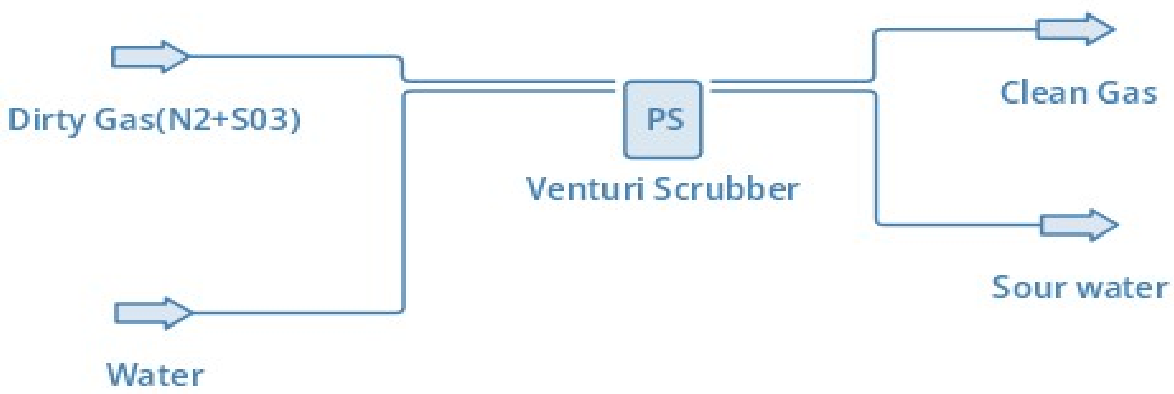
$$\psi = \frac{\rho_p d_p^2 (V_p - V_{d_i})}{9\mu_g d_d} \quad (10)$$

3.4. Dust removal efficiency

The dust removal efficiency is calculated from the following equation,

$$E_{re} = 1 - \frac{C_o}{C_i} = 1 - exp\left[-\frac{3}{2}\frac{Q_l}{Q_g}\frac{x}{d_d}\frac{v_d}{v_g - v_d}\eta\right] \quad (11)$$

4.5 Simulation Procedure and Flowsheet:



The venturi scrubber was simulated in **DWSIM using IronPython scripting** to model the gas–liquid interaction and evaluate the particle collection efficiency. The simulation integrates thermodynamic properties obtained from the DWSIM flowsheet with mathematical correlations describing droplet formation and particle capture inside the venturi.

First, the **geometrical parameters of the venturi scrubber** were defined as input variables. These include the lengths of the converging section, throat section, and diffuser section, along with the throat diameter and venturi length. Additional physical parameters such as particle diameter, particle density, surface tension of the liquid, gas velocity, droplet velocity, and inlet particle concentration were also specified. These parameters describe the operating conditions of the venturi scrubber and are required for modelling droplet formation and collection efficiency.

Next, the **process streams were obtained from the DWSIM flowsheet**. Two inlet streams were considered: the contaminated gas stream and the scrubbing liquid stream (water). Using built-in DWSIM property functions, important thermophysical properties such as heat capacity, thermal conductivity, density, viscosity, temperature, flow rate, and composition were extracted from both streams. These properties are required to calculate flow characteristics and droplet behaviour inside the scrubber.

After obtaining the stream properties, the **volumetric flow rates of gas and liquid** were calculated using the ratio of mass flow rate to density. The cross-sectional area of the venturi throat was then determined from the throat diameter. Using the gas and droplet velocities, the **relative velocity between gas and liquid droplets** was calculated, which is an important parameter influencing particle capture.

The next step involved estimating the **diameter of the droplets formed in the venturi throat**. A correlation involving surface tension, liquid viscosity, liquid flow rate, and gas flow rate was used to determine the droplet size produced due to atomization of the liquid at high gas velocities. This droplet diameter determines the available surface area for particle collection.

Following this, the **dimensionless impaction parameter** was calculated using particle properties, gas viscosity, droplet diameter, and relative velocity between gas and droplets. From this parameter, the **single droplet collection efficiency** was determined using an empirical efficiency correlation. This efficiency represents the probability that a particle collides with and attaches to a liquid droplet.

Finally, the **outlet particle concentration** was estimated using an exponential removal model that considers liquid-to-gas flow ratio, venturi length, droplet size, and collection efficiency. Using the inlet and outlet particle concentrations, the **overall dust removal efficiency of the venturi scrubber** was calculated.

The simulation results were displayed in the DWSIM message window, including the **diameter of droplets formed in the venturi, single droplet collection efficiency, and overall dust removal efficiency**. These results help evaluate the performance of the venturi scrubber under the specified operating conditions.

particle removal efficiency, providing a useful model for analysing the performance of venturi scrubbers in pollution control applications.

4.6 Results and Discussion:(DWSIM Results)

ⓘ	3	3/12/2026 8:34:32 PM	Message	The flowsheet was calculated successfully. [1.978s]
ⓘ	2	3/12/2026 8:34:32 PM	Message	Dust Removal Efficiency= 0.99948657250418071
ⓘ	1	3/12/2026 8:34:32 PM	Message	Single Droplet Efficiency= 0.33375221697939944
ⓘ	0	3/12/2026 8:34:32 PM	Message	Diameter of the droplet in venturi = 0.00089227936814218118m

5.Conclusion

The present study focused on the **modelling and simulation of a fired heater and a venturi scrubber using DWSIM with IronPython scripting**. The objective was to understand the working principles of these important industrial units and to analyze their performance using mathematical models and process simulation tools.

In the case of the **fired heater**, the simulation involved modelling both the **convection and radiant sections** of the heater. Heat transfer calculations, temperature profiles, tube requirements, and pressure drop within the system were evaluated using appropriate correlations. The simulation successfully determined important design parameters such as the **number of radiant tubes, number of convection tubes, and the pressure drop across the heater**. These results help in understanding the heat transfer mechanisms involved in fired heaters and their role in heating process streams in industries such as petroleum refining and petrochemical processing.

For the **venturi scrubber**, the simulation focused on modelling the **gas–liquid interaction responsible for particulate removal**. The droplet formation, relative velocity between gas and liquid droplets, and particle capture mechanisms were analyzed using empirical correlations. The model predicted key performance parameters including the **droplet diameter formed in the venturi throat, single droplet collection efficiency, and overall dust removal efficiency**. These results demonstrate the effectiveness of venturi scrubbers in removing fine particulate matter from industrial gas streams.

Overall, the use of **DWSIM combined with Python scripting** provided a flexible and efficient platform for simulating complex industrial equipment. The study highlights how process simulation can be used to analyze operating conditions, evaluate performance, and understand the behaviour of pollution control and heat transfer equipment. Such simulations are valuable tools for **process design, optimization, and environmental control in chemical and process industries**.

6.References:(Research papers):

A)Dust particle Removal Efficiency of a Venturi Scrubber-Majid Ali,Changqi Yan,Khurram Mehboob.

B)Modelling and Optimization of process fired heater-Mojtaba haratian,Majid Amirpour.