POLITECNICO DI TORINO

DIMEAS - DEPARTMENT OF MECHANICAL AND AEROSPACE ENGINEERING

Master's degree thesis

TOPIC

"Modeling study on the geometry of an ejector for PEM fuel cells using MATLAB and COMSOL"

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Abstract :

A MATLAB-based optimization methodology is developed to enhance the geometry of ejectors in Proton Exchange Membrane (PEM) fuel cells, focusing on improving hydrogen recirculation and fuel utilization efficiency. A custom, non-parametric MATLAB algorithm systematically refined key geometric parameters—including nozzle, throat, and mixing chamber dimensions—to maximize the ejector's entrainment ratio. This ratio is essential for recycling unconsumed hydrogen, enhancing PEM fuel cells' overall efficiency and sustainability.

The MATLAB algorithm employs a surrogate-based optimization approach, enabling rapid iterative adjustments by optimizing control points across the ejector profile. Multiple ejector profiles were evaluated and refined, with Profile 17(C) achieving the highest entrainment ratio among the tested designs. To validate the optimized geometries, high-fidelity COMSOL simulations were used, providing detailed fluid dynamic analysis that closely aligned with MATLAB results and confirmed the algorithm's effectiveness in generating high-performance designs. This integrated MATLAB-COMSOL approach leverages the speed of MATLAB-based optimization with COMSOL's simulation accuracy, creating a robust framework for advanced ejector design.

The study underscores the effectiveness of MATLAB-driven optimization with COMSOL validation in advancing PEM fuel cell technology, particularly through customized ejector configurations that enhance hydrogen efficiency. Future work will expand on this framework by integrating real-world data and machine learning to adapt ejector performance under diverse operational conditions.

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Chapter 1

1. Introduction

1.1 Overview of Fuel Cells

Fuel cells are electrochemical devices that convert chemical energy from a fuel and an oxidizing agent into electrical energy through a pair of redox reactions[1]. These reactions obviate the necessity for burning, hence circumventing pollutants and thermodynamic constraints linked to traditional power production systems [2]. Fuel cells' superior efficiency and minimal environmental effect establish them as an essential technology for various uses, including stationary power production and vehicle propulsion [3]. This adaptability is crucial as global energy requirements transition towards sustainable alternatives [4].

1.2 PEM Fuel Cells

Polymer Electrolyte Membrane (PEM) fuel cells are distinguished by their elevated power density, efficiency, and low operating temperatures, rendering them suitable for transportation applications [5]. Their swift initiation and zero-emission characteristics bolster a hydrogen-centric economy, by climate change mitigation initiatives [6&7]. We expect that PEM fuel cells will substantially aid the shift towards greener energy alternatives, particularly by supplanting conventional combustion engines in the automotive sector [8].

1.3 Challenges in Hydrogen Management

PEM fuel cells have difficulties in maximizing hydrogen utilization. Effective hydrogen recirculation and management systems are vital for maximizing fuel consumption and reducing waste, which is crucial for the performance of fuel cell stacks [9 & 10]. The anode side generally sustains a high hydrogen excess ratio to accommodate fluctuating power requirements, regulate the pressure differential between electrodes, and improve water management inside the stack [11]. Anodic recirculation systems (ARS) recycle hydrogen from the anode exhaust and reintroduced it into the cell. This can enhance fuel efficiency, reduce environmental impact, and increase system efficiency [12].

1.4 Objective of the Study

The Primary objective of this study is to optimize the ejector geometry in anodic recirculation systems (ARS) for Proton Exchange Membrane Fuel Cells (PEMFCs) to significantly improve the entrainment ratio. The entrainment ratio, a crucial parameter that determines the ejector's efficiency in mixing secondary fluid with the primary flow, is essential for assessing the overall performance and efficacy of the ejector. [13 & 14].

The study has an advanced non-parametric optimization approach to iteratively enhance the ejector's critical geometric parameters, including the nozzle, throat, and mixing chamber. This research employs MATLAB-based surrogate modeling for swift optimization and utilizes COMSOL Multiphysics for comprehensive fluid dynamics validation, ensuring designs are both Computationally efficient and physically precise.

This study investigates both the direct effects of geometric modifications on the entrainment ratio and the fundamental fluid dynamics mechanisms that drive these alterations. The results are anticipated to aid in the creation of more efficient ejector designs that optimize entrainment while maintaining operational stability, thus improving the scalability of PEMFC technology for commercial use [11 & 12].

Chapter 2

2. Literature Review

Ejectors are passive devices commonly used across applications like refrigeration, air conditioning, and fluid transport. They operate by utilizing high-pressure fluids to entrain and transport low-pressure secondary fluids without the need for external power sources [12]. In proton exchange membrane fuel cells (PEMFCs), ejectors are very important for recycling hydrogen that hasn't been used up. This improves fuel efficiency and operational effectiveness without adding any extra mechanical parts [13]. However, geometric optimization can significantly improve the performance of ejectors, specifically the entrainment ratio, which measures the effectiveness of mixing and recirculation [6].

2.1 Importance of Ejector Geometry

The geometric configuration of an ejector is essential to its performance. Huang et al. [6] and other studies have shown that changing certain parameters, like the nozzle throat diameter, mixing chamber dimensions, and nozzle exit position, can have a big effect on how well fluids mix and how momentum is transferred inside the ejector. For PEMFC applications, well-designed ejectors must maximize the recycling of unconsumed hydrogen to reduce fuel waste and improve system efficiency [7].

2.2 Ejector Design Optimization Techniques

Numerous studies have explored techniques to optimize ejector performance. Computational Fluid Dynamics (CFD) is frequently employed to simulate fluid flow within ejectors and predict their performance under different geometric configurations [9]. For instance, Yang et al. (2020) [7] investigated multi-nozzle ejectors in PEMFC systems. They showed how important it is to make precise geometric changes to improve both the entrainment ratio and the overall efficiency. This study utilizes surrogate optimization algorithms and non-parametric design methods, which enable the exploration of a wider range of shapes through continuous refinement based on performance feedback, thereby overcoming the limitations of fixed parametric designs [15].

2.3 Geometrical Parameters and Their Impact on Performance

Several geometric factors, including nozzle throat diameter, nozzle exit position (NXP), and the design of the mixing chamber and diffuser, significantly influence ejector performance. The nozzle throat, in particular, dictates the velocity of the primary stream, which in turn affects the efficiency of entraining the secondary fluid [16]. Studies indicate that optimal nozzle design is critical for minimizing flow restrictions and enhancing secondary flow development, ultimately improving the entrainment ratio [15].

2.4 Computational Studies and Simulation Comparisons

Comparative studies utilizing MATLAB and COMSOL multiphysics simulations are valuable for validating optimized designs. MATLAB-based optimization algorithms target specific performance parameters, such as the entrainment ratio, while COMSOL provides a detailed physics-based simulation that captures complex fluid interactions [17]. These tools complement one another, as MATLAB allows for rapid iterative design adjustments, and COMSOL offers high-fidelity validation to ensure the designs are robust and practical for real-world applications [13].

2.5 Future Directions for Ejector Optimization

Emerging research suggests that integrating machine-learning algorithms into the optimization process may achieve further improvements in ejector performance. Machine learning can analyze extensive design spaces more effectively, potentially identifying novel geometries that surpass traditional design limitations [18]. Also, experiments are still needed to make sure that optimized ejectors work well and are reliable, especially when they are used in PEMFC systems with a range of operating conditions [19].

2.6 Ejector Design and Working Principles

An ejector is a mechanical device that uses high-pressure fluid (typically gas or liquid) to entrain and transport a lower-pressure fluid through mixing and momentum transfer [12]. Operating on the Venturi principle, an ejector creates a low-pressure zone through a high-velocity stream, drawing in a secondary fluid. Following their combination, the two streams discharge the mixed fluid at a higher velocity [1].

2.6.1 Working Principle of the Ejector:

The primary function of the ejector is to transform pressure energy into kinetic energy. A high-pressure hydrogen stream from the fuel supply acts as the driving fluid, flowing through a specially designed-nozzle to produce a high-velocity jet. This high-speed jet induces a low-pressure area, effectively drawing in unreacted hydrogen from the anode outlet as the secondary flow. The combined streams then return to the anode, sustaining a continuous fuel flow [6 & 13].

2.6.2 Fluid Dynamics Mechanism:

a. **Primary Flow (Driving Fluid)**: High-pressure hydrogen accelerates through a converging nozzle, increasing in velocity as static pressure decreases, creating the suction effect [16].
b. **Secondary Flow (Entrained Fluid)**: The low-pressure area at the nozzle exit entrains the secondary fluid (unconsumed hydrogen) into the ejector, enabling effective mixing [5].
c. **Mixing Process**: The primary and secondary flows intermix in the mixing chamber, designed to promote uniform velocity distribution and efficient energy exchange [11].
d. **Discharge Phase**: The mixed fluid exits through a diffuser, where high kinetic energy is partially converted back into pressure energy, facilitating reintegration into the fuel cell system [14].

2.6.3 Ejector Geometric Parameters optimization.

The design of an ejector depends on multiple geometric parameters that significantly influence performance, such as nozzle throat diameter, mixing chamber dimensions, diffuser design, and nozzle exit position [7].

I. Ejector Components

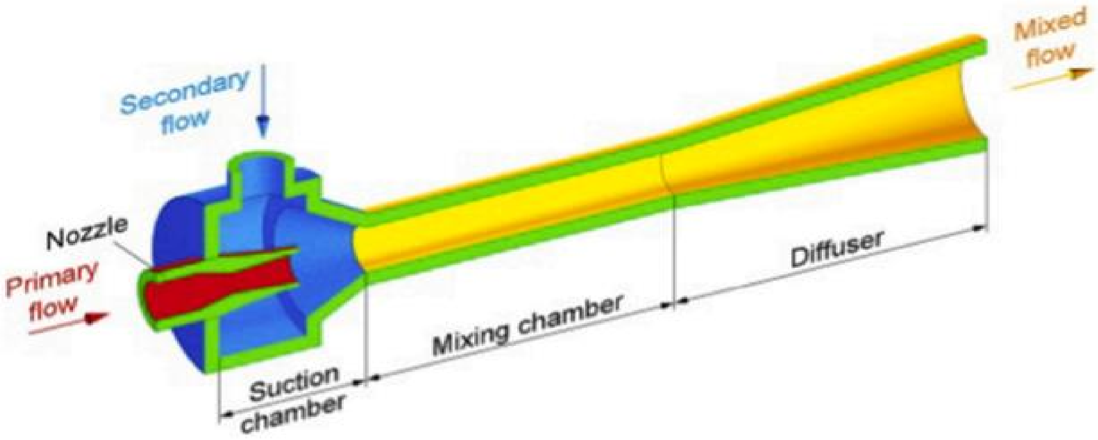

Figure 1 - 3-D structure of an ejector

The structure of an ejector can be broadly categorized into three main components:

a. **Suction Chamber**: Where the secondary fluid enters, establishing conditions for efficient entrainment [9].
b. **Mixing Tube**: This can be configured for constant-pressure mixing (CPM) or constant-area mixing (CAM) to support stable or variable pressure conditions, respectively [6].
c. **Diffuser**: Converts kinetic energy back into pressure, enabling efficient fluid discharge [8].

II. Key Geometric Parameters

1. **Nozzle Throat Diameter**: The nozzle throat diameter is a critical parameter that directly influences the velocity of the primary stream. Reducing the diameter increases the velocity, creating a lower-pressure zone that enhances entrainment but may result in increased flow losses if the diameter is too small [21].

2. **Nozzle Exit Position (NXP)**: The position of the nozzle exit relative to the mixing chamber affects both the critical back pressure and the entrainment ratio. It can be classified as .

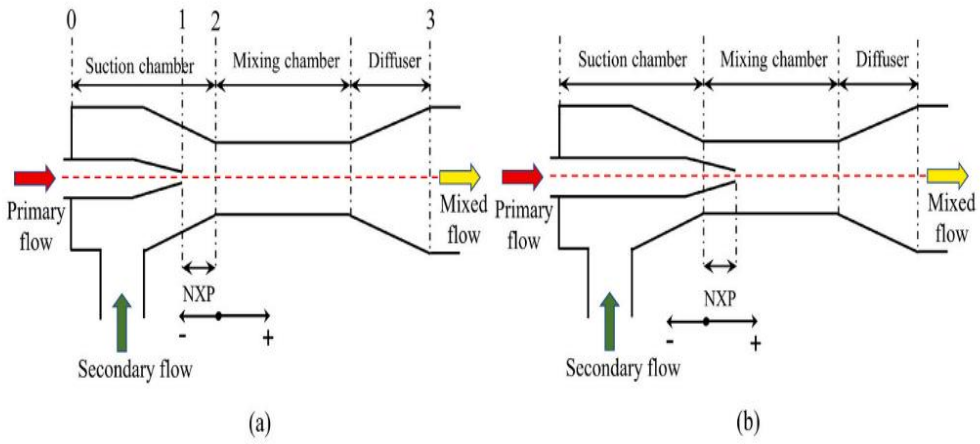

Figure 2 - Two main ejector types: (a) the CPM ejector and (b) the CAM ejector

- **Negative NXP (CPM)**: The nozzle exit is within the suction chamber, allowing for prolonged mixing and better pressure stabilization.
- **Positive NXP (CAM)**: The nozzle exit is at the front of the mixing chamber, which can facilitate faster flow entry but may compromise mixing efficiency [22].

3. **Mixing Chamber Dimensions**: The dimensions of the mixing chamber, particularly its length and diameter, play a key role in mixing efficiency. A longer chamber allows for more thorough mixing but may introduce additional pressure losses.
4. **Diffuser Design**: Diffuser geometry, including angle and length, is critical in managing energy losses. Optimal diffuser design smooths the flow transition from high velocity to higher pressure, reducing turbulence and enhancing ejector efficiency [23].
5. **Inclination of the Secondary Tube**: The angle at which the secondary flow enters the mixing chamber affects how well it integrates with the primary flow. Optimal design should consider the angle of entry to maximize mixing efficiency [18].

III. Entrainment Ratio (ε)

The **entrainment ratio (ε)** is a fundamental metric for evaluating ejector performance, defined as:

$$\varepsilon = \frac{WS}{WP}$$

Where:

- WS = Mass flow rate of the secondary fluid (entrained fluid)
- WP = Mass flow rate of the primary fluid (working fluid)

This ratio provides insight into the efficiency with which the ejector entrains the secondary flow, and it is influenced by various design parameters [18].

IV. Operating Conditions

The operational conditions significantly affect ejector performance. Key factors include:

- **Mass Flow Rate**: The flow rates of both primary and secondary fluids determine the operational efficiency of the ejector. Variations can lead to fluctuations in entrainment and overall performance.
- **Temperature and Humidity**: The properties of hydrogen, such as viscosity and density, are temperature and humidity dependent. Designing ejectors to accommodate varying conditions is essential for maintaining efficiency.

V. Advanced Fluid Dynamics Considerations

Understanding the advanced fluid dynamics principles governing ejector operation is vital for optimizing design and enhancing performance.

a. Bernoulli's Principle

Bernoulli's equation, which describes the conservation of energy in fluid flow, is fundamental in analyzing ejector behavior. It states that an increase in fluid velocity leads to a corresponding decrease in pressure, thus providing the theoretical foundation for the suction effect observed in ejectors [25].

b. Continuity Equation

The **continuity equation** governs the conservation of mass within the ejector. It ensures that the mass flow rates before and after the mixing chamber remain constant, which is crucial for achieving desired entrainment ratios and maintaining system efficiency [25].

c. Navier-Stokes Equations

The **Navier-Stokes equations** are pivotal in understanding the behavior of viscous fluids. While simplified models may be sufficient for basic design, incorporating these equations in computational fluid dynamics (CFD) simulations can yield insights into complex flow phenomena, including:

- **Shock Waves**: Rapid changes in pressure and density that can occur in high-speed flows.
- **Vortex Formation**: Regions of swirling flow that can arise from improper nozzle exit positioning or excessive secondary flow velocity.
- **Boundary Layer Effects**: The layer of fluid in the vicinity of the ejector surfaces, which can significantly influence drag and overall flow efficiency [24].

3. Methodology for Ejector Optimization

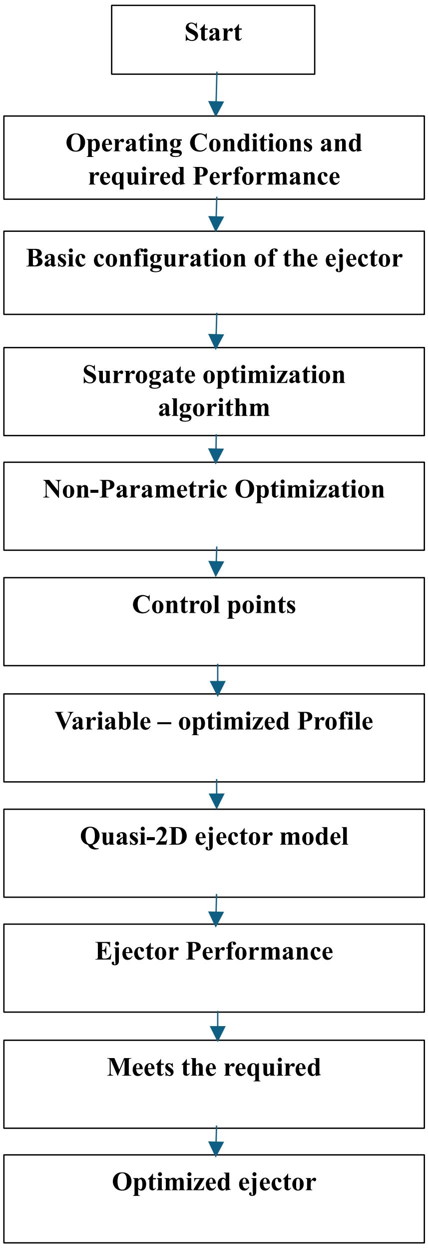

Figure 3 - Flow-chart of the collaborative design optimization method for ejectors used in this study.

3.1 Optimization Process Overview:

The flowchart shows the process of improving the design of an ejector in a proton exchange membrane (PEM) fuel cell system. It starts with setting up the operating conditions and ends with a profile for the ejector that works best. Below is a detailed step-by-step explanation of each stage in the process [6].

a. **Start**: This marks the beginning of the optimization process, indicating the initiation of the ejector design and evaluation journey [6].
b. **Operating Conditions and Required Performance**: At this stage, the operating parameters, such as pressure, temperature, and flow rate, along with the desired performance targets (e.g., entrainment ratio, efficiency) of the ejector are defined. These conditions guide the subsequent design process [6].
c. **Basic Configuration of the Ejector**: The operating conditions dictate the development of the ejector's fundamental geometric structure. This includes determining initial design elements such as the nozzle, throat, and mixing chamber sizes [6].
d. **Surrogate Optimization Algorithm**: use a surrogate model to optimize the design more efficiently. This model approximates the performance of the ejector using mathematical algorithms, enabling faster iterations and evaluations without the need for full-scale simulations at every step [6].
e. **Non-Parametric Optimization**: At this stage, the optimization concentrates on non-parametric variables, which means that predefined parameter limits do not constrain the design. Instead, it explores a broader range of shapes and configurations to improve performance [6].
f. **Control Points**: We make adjustments to optimize the shape at specific locations within the ejector geometry, known as control points. The optimization process modifies the geometry based on these points [6].
g. **Variable-Optimized Profile**: We create a variable-optimized profile after adjusting the control points. This is the initial form of the ejector, which emerges from the optimization process and reflects modifications in the geometry to enhance performance[6].
h. **Quasi-2D Ejector Model**: This step evaluates the optimized ejector profile using a quasi-2D model, transforming the 3D structure into a two-dimensional framework to speed up

computations. This model simulates fluid flow to assess the performance of the optimized geometry [6].

i. **Ejector Performance**: We test the optimized ejector's performance against key metrics such as the entrainment ratio and pressure losses to verify if the improvements meet the desired targets. [6].

j. **Meets the Required**: The process moves forward if the optimized ejector meets the required performance criteria, such as achieving the desired entrainment ratio and flow efficiency[6].

k. **Optimized Ejector**: The optimized ejector has undergone rigorous testing and adjustment through simulation, confirming its final design at this stage [6].

l. **End**: The process concludes with a validated and optimized ejector design that meets the required operational and performance standards [6].

In summary, this flowchart outlines an iterative process of defining conditions, configuring the ejector, and using optimization algorithms and simulations to arrive at a highly efficient, custom-designed ejector for use in fuel cell systems [6].

3.1.1 Basic configuration of the ejector.

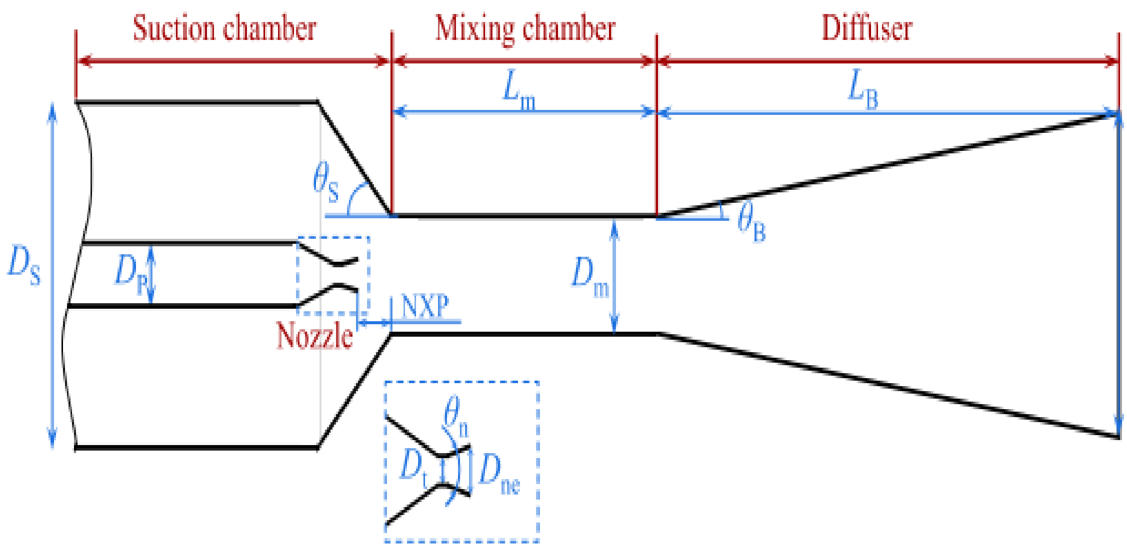

Figure 4 - Schematic of the structure of a fuel ejector.

Table 1- Structural parameters of the basic ejector

Structural parameter	Value
D_P	5mm
D_S	25mm
D_t	0.5mm
Θ_n	10.4°
D_{ne}	0.73mm
NXP	4.3mm
Θ_m	14.7°
D_m	3.61mm
L_m	25.9mm
D_B	17mm
L_B	85.4mm

Abbreviations:

D_S, diameter of the secondary flow inlet (suction chamber)

D_P, diameter of the primary flow inlet

θ_S, suction chamber convergence angle

NXP, nozzle exit position

L_m, length of the mixing chamber

D_m, diameter of the mixing chamber

θ_B, diffuser angle

L_B, length of the diffuser

D_t, diameter of the nozzle throat

θ_n, nozzle divergence angle

D_{ne}, diameters of the nozzle exit. [6].

Table 2- Optimized ejector operating conditions.

T_p (°C)	P_p (MPa)	T_s (°C)	P_s (MPa)	P_B (MPa)
250	0.585	150	0.0989	0.1031,0.1035,0.1038

Abbreviations:

T_p, Primary Temperature of working fluid

P_p, Primary pressure of working fluid

T_s, Secondary Temperature of working fluid

$P_{s,}$ Secondary pressure of working fluid

$P_{B,}$ Ejector outlet Pressure of working fluid. [6].

3.1.2 Non-parametric optimal design method for ejectors

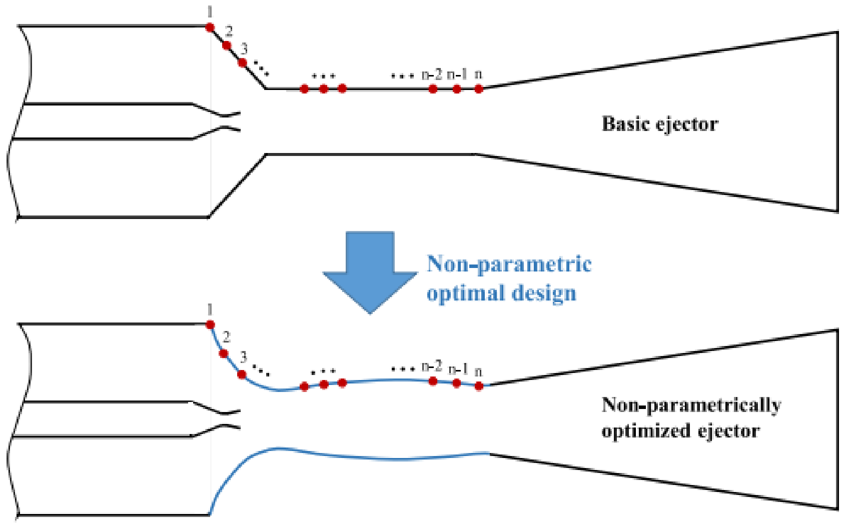

Figure 5- Schematic of a non-parametric optimal design method for ejectors, where n is the number of control point.

In a non-parametric optimization approach, the design of the ejector is not limited by predefined or fixed structural parameters, as in traditional parametric optimization. Instead, it allows for greater flexibility in shaping the ejector's profile by employing control points [6].

a. **Control Points**:

- In this method, n control points are positioned along the longitudinal axis of the ejector. These control points are essentially adjustable reference markers that define the ejector's shape.
- The longitudinal coordinates (x-axis positions) of these control points are optimized during the process. By adjusting the location of each point, the geometry of the ejector can be tuned.

b. **Profile Formation**:

- Once the control points are positioned, the ejector profile is created by connecting these control points through interpolation. Interpolation is a mathematical technique that smooths out the curve between control points, resulting in an arbitrary curved profile. This method provides a fluid, continuous curve that defines the overall shape of the ejector, allowing for fine-tuned adjustments without being limited to fixed parameters such as predefined diameters or lengths.

c. **Arbitrare Shape**:

- The ability to optimize the **arbitrary curved profile** makes this approach highly adaptable. The **profile shape** can be continuously refined to improve performance. This flexibility means that the geometry is not constrained to specific shapes (such as a conical or cylindrical profile), giving the optimizer a broader design space to explore.

d. **Variable Number of Optimization Variables**:

- One of the key advantages of this method is that the number of optimization variables can theoretically approach infinity. This means that more control points can be added as needed, further increasing the ability to adjust the ejector's profile. However, in practice, the number of control points must be carefully managed to balance computational efficiency and design flexibility.

3.1.3 Surrogate Optimization Algorithm

To solve the optimization problem globally, a surrogate optimization algorithm is employed.

a. **Global Optimization**:

- Surrogate optimization is a global optimization technique that is used to explore the entire design space and identify the optimal solution. It does this by building a simplified model (or surrogate) of the real function being optimized (in this case, the performance of the ejector) [20].
- The surrogate model approximates the actual performance metrics (e.g., entrainment ratio) based on the control points, allowing the algorithm to evaluate potential designs more quickly than if it had to rely on full-scale simulations or experiments at each iteration [20].

b. **MATLAB v.2020b Optimization Toolbox**:

- The surrogate optimization algorithm used in this approach is part of the MATLAB v.2020b Optimization Toolbox, which provides advanced tools for global optimization. MATLAB's built-in functions streamline the process of running the optimization loop, handling complex variable interactions, and managing constraints on the control points [20].

c. **Efficient Design Optimization**:

- By using this global algorithm, the optimization process becomes more efficient. The algorithm avoids local optima (suboptimal solutions that are optimal only within a small region of the design space) and works toward finding the global optimum (the best possible solution in the entire design space). This ensures that the ejector design achieves maximum efficiency in terms of performance [20].

3.2 MATLAB Algorithm for Ejector Shape Optimization

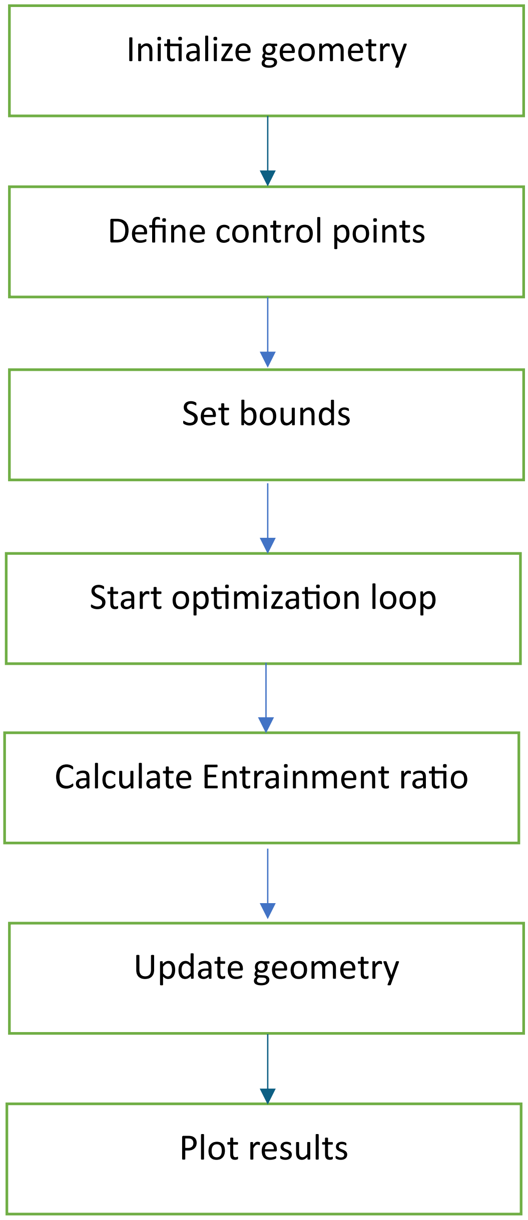

figure 6 - Workflow for Ejector Shape Optimization Using MATLAB Algorithm.

The program flowchart provides a detailed, step-by-step process for optimizing the geometry of an ejector, particularly focusing on maximizing the entrainment ratio—the key metric for ejector performance. Here is a more in-depth explanation of each stage in the flowchart:

a. Initialize Geometry

- In this first step, establish the initial design of the ejector. It involves setting up a base configuration, which includes defining the key geometric parameters, such as the nozzle diameter, throat length, and mixing chamber dimensions. This geometry serves as the starting point for the optimization process.
- The geometry may be based on prior knowledge, theoretical models, or an arbitrary starting shape. Importantly, this initial geometry may not be optimal and is subject to change as the optimization progresses [20].

b. Define Control Points

- The optimization process will adjust specific locations or variables in the geometry, known as control points. These control points could represent critical geometric aspects like the curvature of the nozzle, the position and diameter of the throat, or the angle of the diffuser.
- The control points essentially define the design space—the areas of the ejector geometry that are adjustable. They often select them based on their sensitivity to performance metrics (like entrainment ratio), implying that changes at these points will significantly influence the ejector's function [20].

c. Set Bounds

- This stage involves defining the constraints or limits for each control point. The bounds define the range in which we can modify the control points. For instance, we might allow the throat diameter to vary between 2 mm and 4 mm, but not beyond those limits.
- These constraints ensure that the optimization stays within feasible and physically realistic designs. Setting bounds is crucial for preventing impractical solutions and ensuring the final design adheres to manufacturing or operational limitations [20].

d. Start Optimization Loop

- At this point, the optimization algorithm begins its work. The algorithm can be based on different methods, such as genetic algorithms, gradient descent, or surrogate modeling. The goal is to iteratively adjust the control points (within the bounds) to improve the ejector's performance.

- The loop refers to the repeated process of adjusting control points, calculating performance (such as the entrainment ratio), and making further adjustments based on the results. This iterative process continues until the performance meets the desired criteria or no further improvement is possible [20].

e. Calculate Entrainment Ratio

- Each iteration of the optimization loop calculates the entrainment ratio. This ratio is an important measure of how well the ejector is working because it shows how much secondary flow (like recirculated hydrogen) is mixed with primary flow (high-pressure hydrogen).
- A higher entrainment ratio indicates better performance, meaning more unreacted hydrogen from the anode exhaust is being recycled back into the fuel cell, which improves efficiency and reduces waste.
- This calculation may involve mathematical models to predict the fluid flow inside the ejector based on its current geometry.

f. Update Geometry

- The optimization algorithm updates the geometry by adjusting the control points based on the calculated entrainment ratio. The optimization algorithm guides this adjustment, aiming to enhance the entrainment ratio through targeted modifications to the ejector's shape and dimensions.
- For instance, if the current geometry doesn't allow for a good entrainment ratio, the algorithm might change the nozzle diameter or throat length to make the mixing of primary and secondary flows better. These updates are crucial to converging toward an optimal design.

g. Plot Results

- In this final step, the results of the optimization process are visualized. Typically, this entails creating plots that illustrate the evolution of the geometry throughout the optimization process and the changes in key performance metrics, like the entrainment ratio, as the geometry underwent refinement.

- The results help determine the success of the optimization process. This step may include visualizations like:

  a. There are graphs showing the entrainment ratio throughout the iterations.
  b. The original and optimized shapes are displayed in geometry plots.
  c. Performance comparisons to see how the new design improves fuel efficiency and system performance.

The process selects the final optimized geometry if the results are satisfactory. If not, the process may return to the optimization loop for further refinement.

Chapter 4

4. Results & Discussion

4.1 Performance of Optimized Profiles

This study tested a total of 10 ejector profiles, specifically focusing on their entrainment ratios, to evaluate their performance. Each profile is characterized by distinct geometric features defined by specific control points that play a crucial role in shaping the ejector's nozzle and mixing chamber. These control points directly influence fluid flow characteristics, impacting overall performance metrics.

4.1.1 Number of Profiles Selection:

- **Exploration of Design Space**: Ten profiles provide a balance between sufficiently exploring the design space and maintaining computational efficiency. Fewer profiles might not capture the full range of potential geometries, while significantly more profiles could lead to diminishing returns without meaningful performance improvements.
- **Optimization Process**: Using 10 profiles made it possible to compare performance metrics (like the entrainment ratio) across different ejector geometries in a structured way. This helped find the configurations that had the best balance between flow efficiency and complexity.
- **Computational Feasibility**: Given the computational resources available, optimizing and validating more than 10 profiles would have required excessive computational time, especially when using MATLAB for iterative optimization and COMSOL for detailed simulations.

4.1.2 Distinctiveness of the Profiles:

- **Geometric Variation**: Each profile has different geometric configurations defined by the placement and manipulation of control points, which influence key parameters like nozzle diameter, throat length, and mixing chamber dimensions. We specifically designed these variations to explore the impact of different geometrical parameters on the entrainment ratio.
- **Performance Comparison**: I measured and compared the profiles' differing entrainment ratios and performance outcomes. For example, in your results, Profile 17(C) had the

highest entrainment ratio, while other profiles exhibited different behaviors due to their unique geometric features.

- **Control Points Influence**: The distinct profiles were determined by the specific adjustments made to control points, which influenced the ejector's ability to entrain and mix the primary and secondary flows. Each profile represents a unique approach to solving the optimization problem, making it crucial for the shape optimization algorithm.

Table 3 - Structural Parameters of the Optimized Ejector for 10 Profiles

Profile	NXP (mm)	L_m (mm)	L_B (mm)	D_t (mm)	D_{ne} (mm)	D_{bo} (mm)	D_{bi} (mm)	D_p (mm)	D_s (mm)
17(A)	4.3	25.9	85.4	2	2.4	23	19.6	12	40
17(B)	4.3	25.9	85.4	2	2.4	23	19.6	12	40
17(C)	4.3	25.9	85.4	2	2.4	23	19.6	12	40
17(D)	4.3	25.9	85.4	0.5	0.62	23	9.4	5.34	32
17(E)	4.3	25.9	85.4	0.8	1.2	23	19.6	8	40
17(F)	4.3	25.9	85.4	1	1.46	21	16.4	10	36
18(A)	4.3	25.9	85.4	2	2.4	25	19.6	12	40
18(B)	4.3	25.9	85.4	2	2.4	25	19.6	12	40
19(A)	4.3	25.9	85.4	2	2.4	25	19.6	12	40
19(B)	4.3	25.9	85.4	2	2.4	25	19.6	12	40

Abbreviations:

NXP - (nozzle exit position)

L_m - (length of the mixing chamber)

L_B - (length of the diffuser)

D_t - (diameter of the nozzle throat)

D_{ne} - (diameters of the nozzle exit)

D_{bo} - (diameter of the diffuser outlet)

D_{bi} - (diameter of the diffuser inlet)

D_p - (Diameter of the Primary flow inlet)

D_s - (Diameter of the secondary flow inlet

1. Ejector Profile 17(A) :

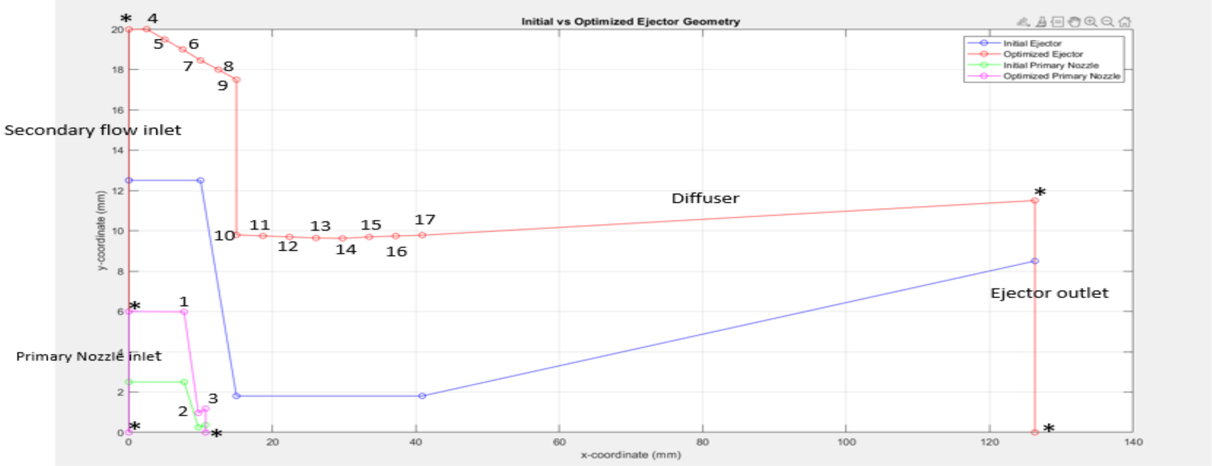

Figure 7 - Ejector Profile 17(A)

Optimized Ejector Entrainment ratio (ER) = 6.34

Table 4 - Optimized Control Points for the Ejector Geometry in Profile 17(A)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	5
	2	19.5	6
	3	18.5	7.5
	4	18	10
	5	17.5	12.5
	6	17	15
Mixing Chamber	1	9.775	15
	2	9.742	18.7
	3	9.667	22.4
	4	9.618	26.1
	5	9.644	29.8
	6	9.681	33.5
	7	9.733	37.2
	8	9.741	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 6 control points to manage fluid intake.
- **Mixing Chamber**: 8 control points to optimize fluid mixing.

2. Ejector Profile 17(B) :

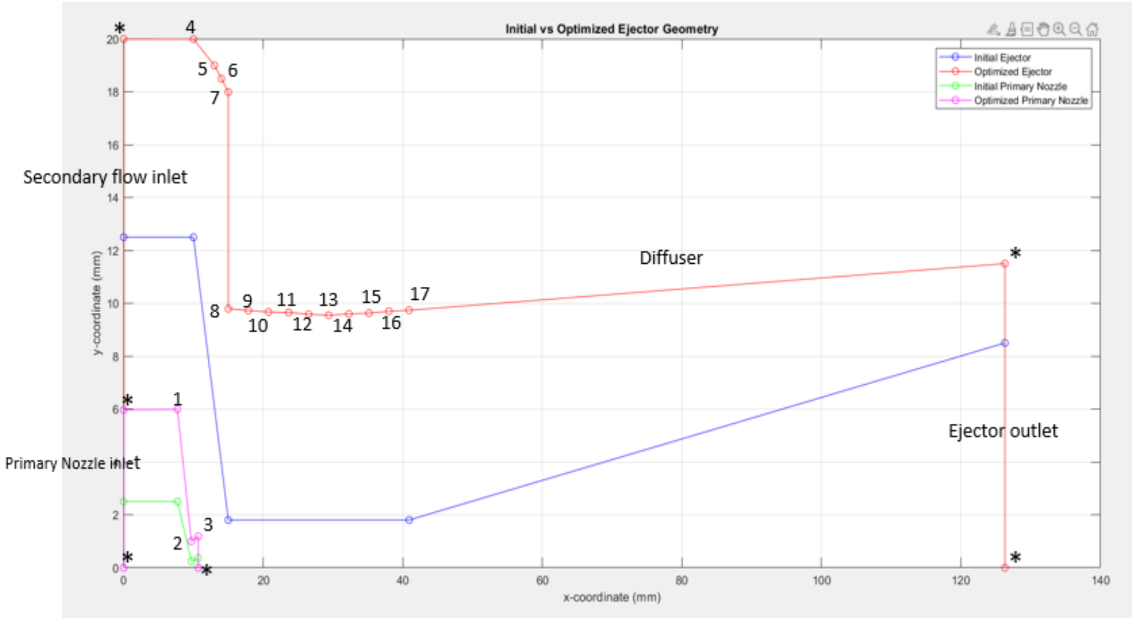

Figure 8 - Ejector Profile 17(B)

Optimized Ejector Entrainment ratio (ER) = 6.16

Table 5 - Optimized Control Points for the Ejector Geometry in Profile 17(B)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	10
	2	19	13
	3	18.5	14
	4	18	15
Mixing Chamber	1	9.8	15
	2	9.727	17.88
	3	9.691	20.76
	4	9.648	23.63
	5	9.6	26.51
	6	9.53	29.4
	7	9.577	32.77
	8	9.638	35.14
	9	9.697	38.02
	10	9.741	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 4 control points to manage fluid intake.
- **Mixing Chamber**: 10 control points to optimize fluid mixing.

3. Ejector Profile 17(C) :

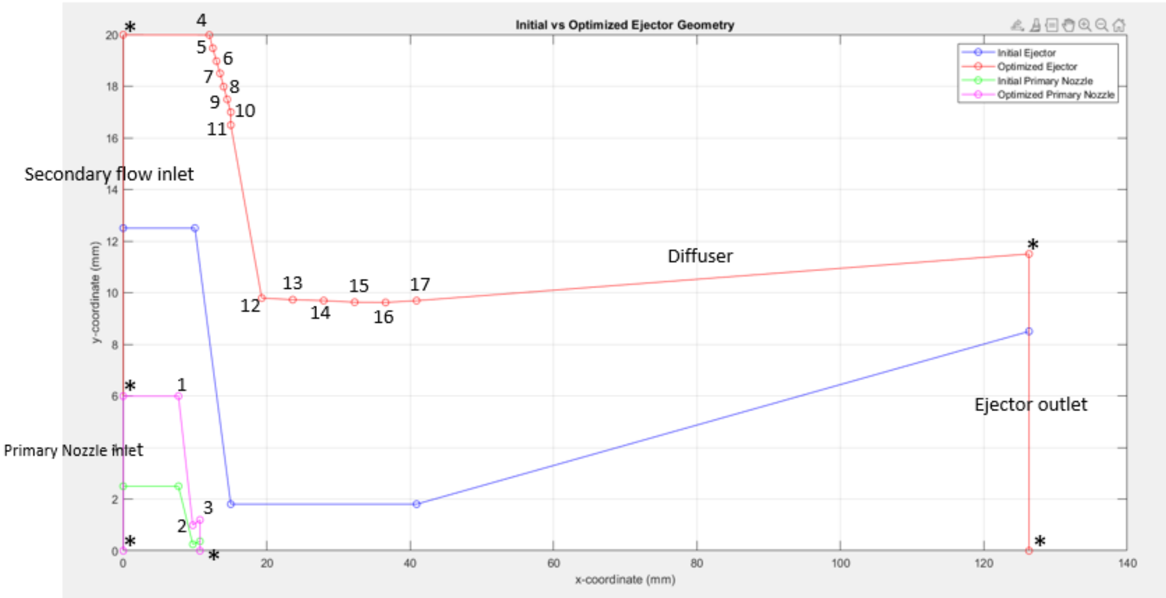

Figure 9 - Ejector Profile 17(C)

Optimized Ejector Entrainment ratio (ER) = 6.48

Table 6 - Optimized Control Points for the Ejector Geometry in Profile 17(C)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	12
	2	19.5	12.5
	3	19	13
	4	18.5	13.5
	5	18	14
	6	17.5	14.5
	7	17	15
	8	9.8	15
Mixing Chamber	1	9.75	19.32
	2	9.7	23.63
	3	9.65	27.95
	4	9.65	32.27
	5	9.7	36.58
	6	9.75	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 8 control points to manage fluid intake.
- **Mixing Chamber**: 6 control points to optimize fluid mixing.

4. Ejector Profile 17(D) :

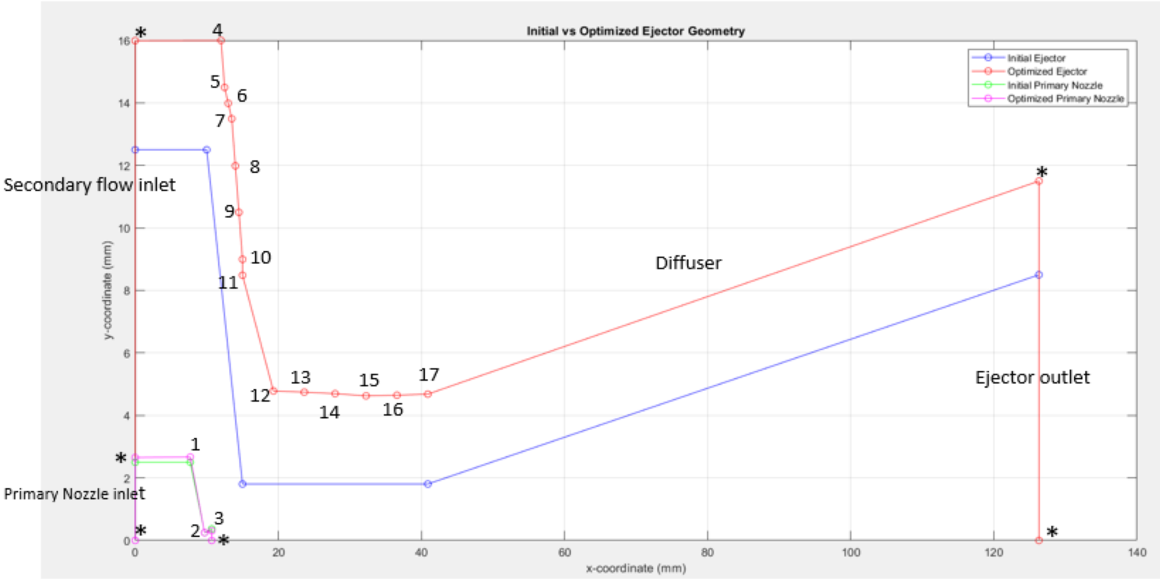

Figure 10 - Ejector Profile 17(D)

Optimized Ejector Entrainment ratio (ER) = 5.58

Table 7 - Optimized Control Points for the Ejector Geometry in Profile 17(D)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	2.67	7.7
	2	0.25	9.7
	3	0.31	10.7
Suction Chamber	1	16	12
	2	14.5	12.5
	3	14	13
	4	13.5	13.5
	5	12	14
	6	10.5	14.5
	7	9	15
	8	8.5	15
Mixing Chamber	1	4.8	19.32
	2	4.745	23.63
	3	4.7	27.95
	4	4.638	32.27
	5	4.627	36.58
	6	4.7	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 8 control points to manage fluid intake.
- **Mixing Chamber**: 6 control points to optimize fluid mixing.

5. Ejector Profile 17(E) :

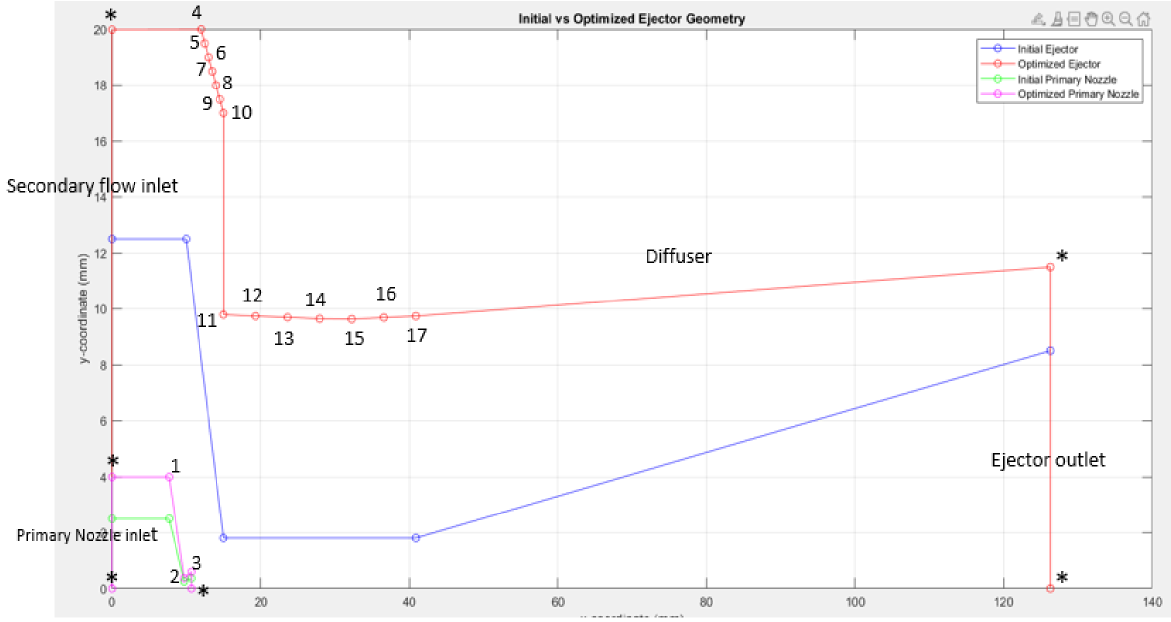

Figure 11 - Ejector Profile 17(E)

Optimized Ejector Entrainment ratio (ER) = 6.36

Table 8- Optimized Control Points for the Ejector Geometry in Profile 17(E)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	4	7.7
	2	0.4	9.7
	3	0.6	10.7
Suction Chamber	1	20	12
	2	19.5	12.5
	3	19	13
	4	18.5	13.5
	5	18	14
	6	17.5	14.5
	7	17	15
Mixing Chamber	1	9.8	15
	2	9.75	19.32
	3	9.7	23.63
	4	9.65	27.95
	5	9.65	32.27
	6	9.7	36.58
	7	9.75	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 7 control points to manage fluid intake.
- **Mixing Chamber**: 7 control points to optimize fluid mixing.

6. Ejector Profile 17(F) :

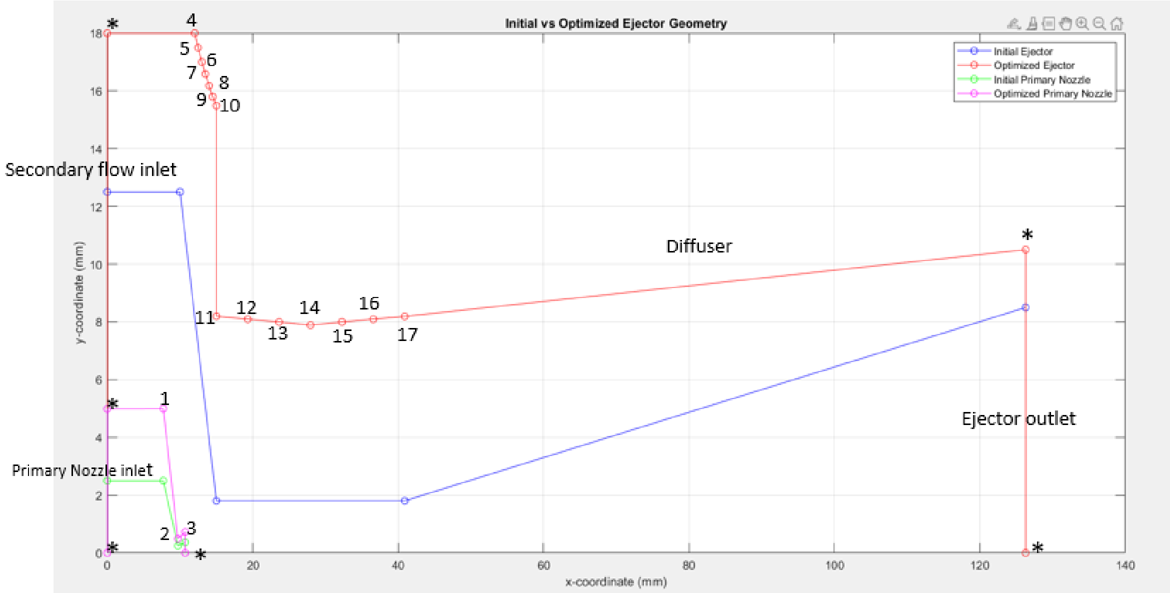

Figure 12 - Ejector Profile 17(F)

Optimized Ejector Entrainment ratio (ER) = 6.12

Table 9 - Optimized Control Points for the Ejector Geometry in Profile 17(F)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	5	7.7
	2	0.5	9.7
	3	0.73	10.7
Suction Chamber	1	18	12
	2	17.5	12.5
	3	17	13
	4	16.6	13.5
	5	16.2	14
	6	15.8	14.5
	7	15.5	15
Mixing Chamber	1	8.2	15
	2	8.1	19.32
	3	7.95	23.63
	4	7.882	27.95
	5	7.907	32.27
	6	8.1	36.58
	7	8.2	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 7 control points to manage fluid intake.
- **Mixing Chamber**: 7 control points to optimize fluid mixing.

7. Ejector Profile 18(A) :

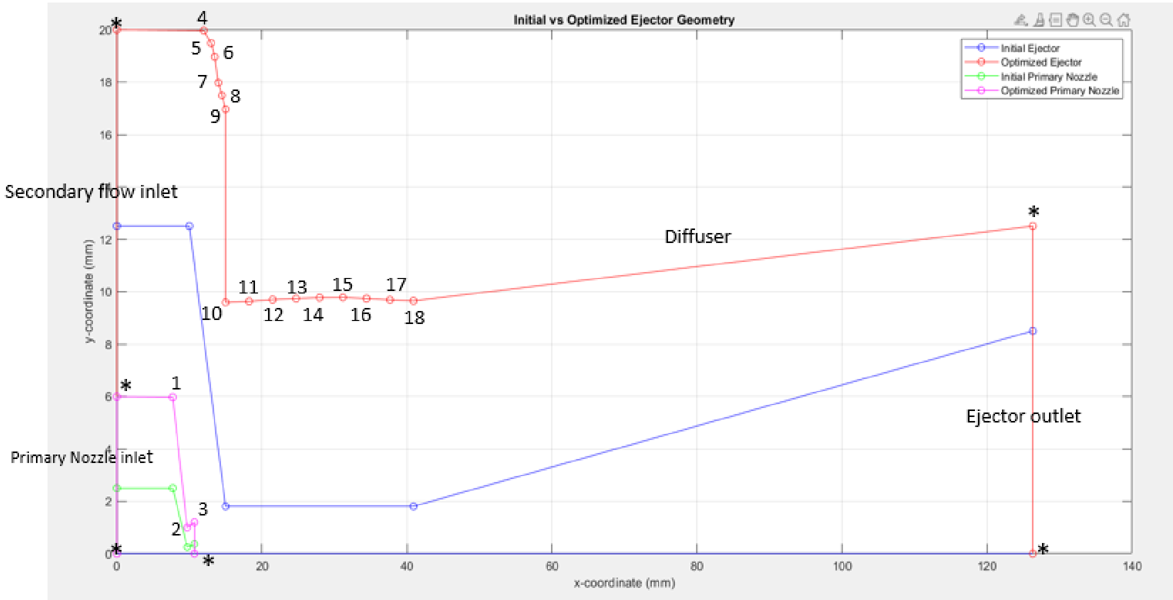

Figure 13 - Ejector Profile 18(A)

Optimized Ejector Entrainment ratio (ER) = 6.42

Table 10- Optimized Control Points for the Ejector Geometry in Profile 18(A)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	12
	2	19.5	13
	3	19	13.5
	4	18	14
	5	17.5	14.5
	6	17	15
Mixing Chamber	1	9.6	15
	2	9.637	18.24
	3	9.664	21.48
	4	9.739	24.71
	5	9.776	27.95
	6	9.786	31.19
	7	9.722	34.42
	8	9.698	37.66
	9	9.647	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 6 control points to manage fluid intake.
- **Mixing Chamber**: 9 control points to optimize fluid mixing.

8. Ejector Profile 18(B) :

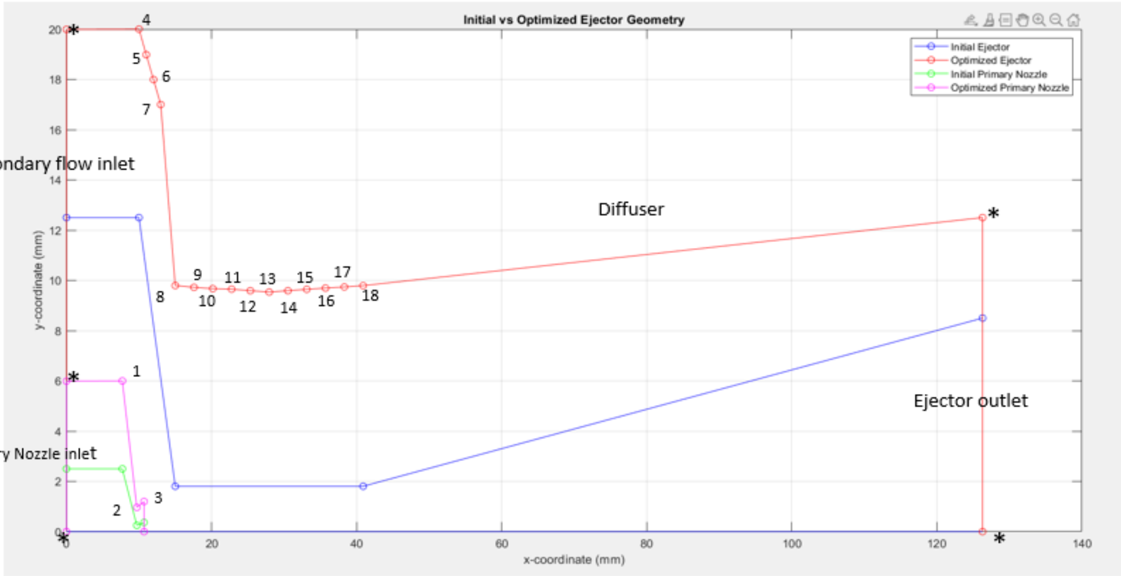

Figure 14 - Ejector Profile 18(B)

Optimized Ejector Entrainment ratio (ER) = 6.26

Table 11- Optimized Control Points for the Ejector Geometry in Profile 18(B)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	10
	2	19	11
	3	18	12
	4	17	13
Mixing Chamber	1	9.8	15
	2	9.792	17.59
	3	9.672	20.18
	4	9.632	22.77
	5	9.594	25.36
	6	9.533	27.95
	7	9.59	30.54
	8	9.621	33.13
	9	9.7	35.72
	10	9.725	38.31
	11	9.77	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 4 control points to manage fluid intake.
- **Mixing Chamber**: 11 control points to optimize fluid mixing.

9. Ejector Profile 19(A) :

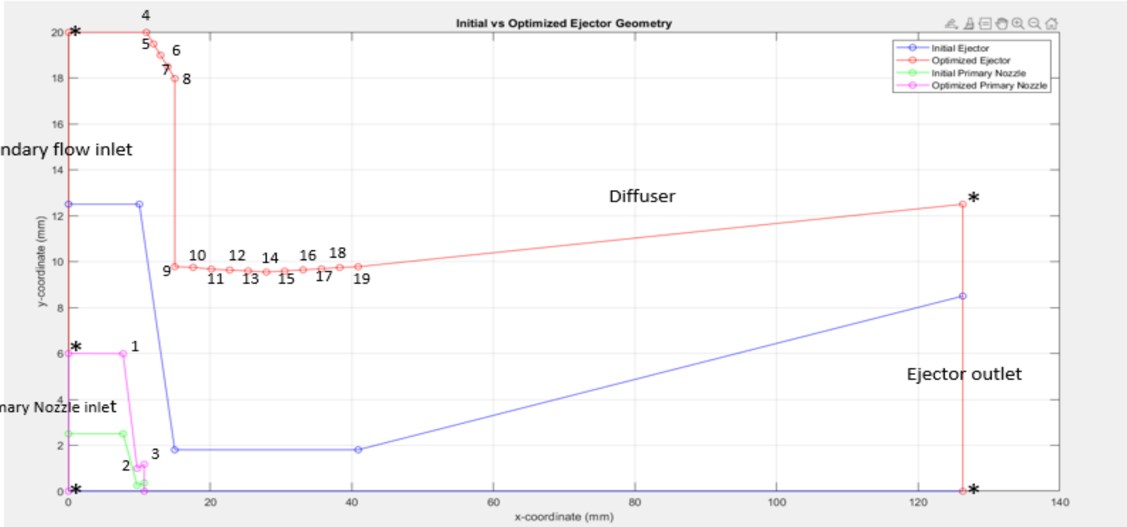

Figure 15 - Ejector Profile 19(A)

Optimized Ejector Entrainment ratio (ER) = 6.45

Table 12 – Optimized Control Points for the Ejector Geometry in Profile 19(A)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	11
	2	19.5	12
	3	19	13
	4	18.5	14
	5	18	15
Mixing Chamber	1	9.8	15
	2	9.70	17.59
	3	9.685	20.18
	4	9.644	22.77
	5	9.575	25.36
	6	9.55	27.95
	7	9.6	30.54
	8	9.6	33.13
	9	9.7	35.72
	10	9.75	38.31
	11	9.8	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 5 control points to manage fluid intake.
- **Mixing Chamber**: 11 control points to optimize fluid mixing.

10. Ejector Profile 19(B) :

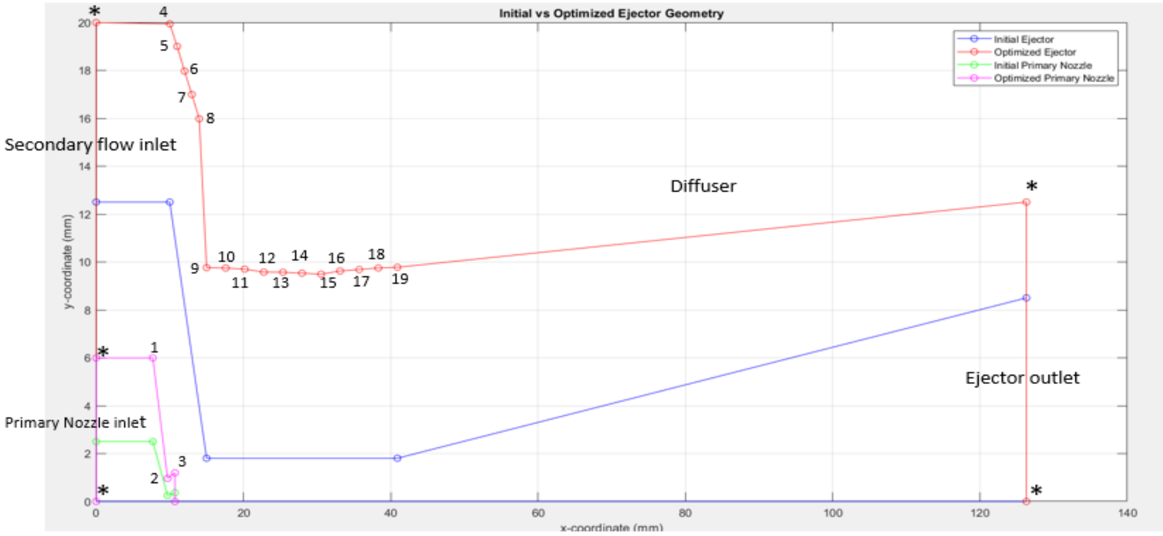

Figure 16 - Ejector Profile 19(B)

Optimized Ejector Entrainment ratio (ER) = 6.4

Table13 – Optimized Control Points for the Ejector Geometry in Profile 19(B)

Chamber	Control Point	x-coordinate (mm)	y-coordinate (mm)
Primary Nozzle	1	7.7	6
	2	9.7	1
	3	10.7	1.2
Suction Chamber	1	20	10
	2	19	11
	3	18	12
	4	17	13
	5	16	14
Mixing Chamber	1	9.789	15
	2	9.748	17.54
	3	9.696	20.18
	4	9.639	22.77
	5	9.572	25.36
	6	9.547	27.95
	7	9.589	30.54
	8	9.642	33.13
	9	9.694	35.72
	10	9.725	38.31
	11	9.78	40.9

Summary

- **Primary Nozzle**: 3 control points to define the shape and geometry.
- **Suction Chamber**: 5 control points to manage fluid intake.
- **Mixing Chamber**: 11 control points to optimize fluid mixing.

4.2 Performance Comparison

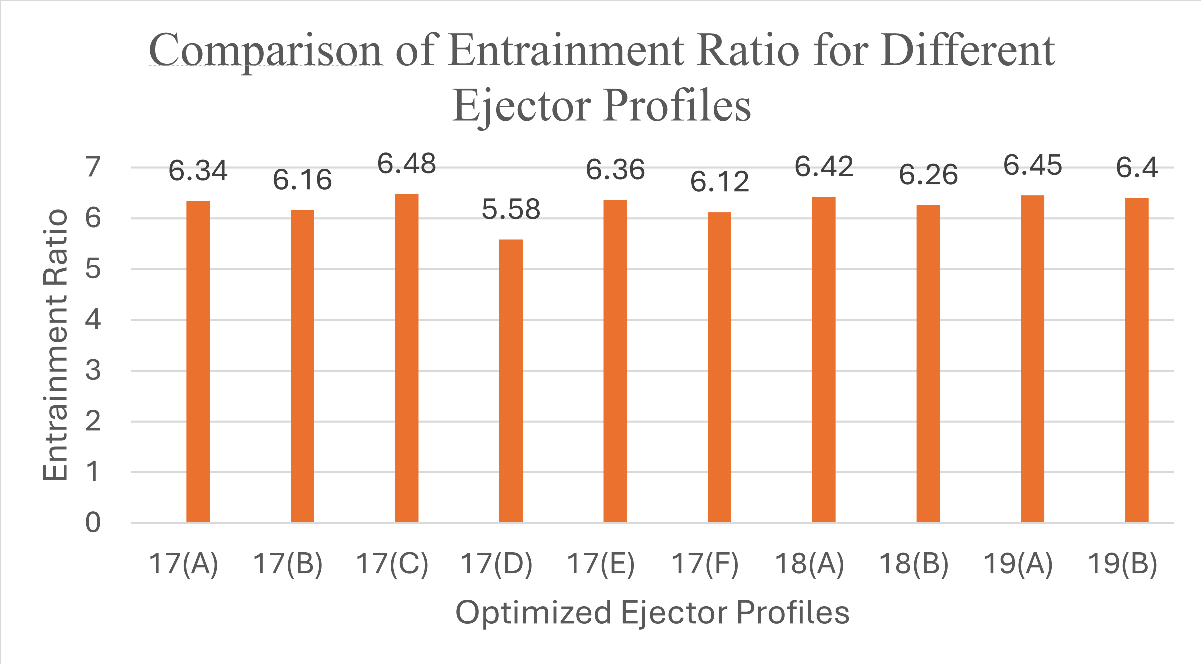

Figure 17 - Entrainment Ratio Comparison for Various Optimized Ejector Profiles.

Best Performing Ejector Profile:

Profile 17(C) demonstrated the best result with an entrainment ratio of **6.48**. This makes it the most efficient profile among the ten tested designs.

4.3 Analysis

- **Geometric Optimization**: Profile 17(C) achieves superior performance due to the optimal arrangement of its control points, specifically in the primary nozzle, suction chamber, and mixing chamber. These control points directly influence the ejector's geometry, which is critical for enhancing the performance by improving flow characteristics and reducing energy losses.
- **Primary Nozzle and Suction Chamber**: In Profile 17(C), we adjusted the control points in the primary nozzle and suction chamber to achieve an ideal balance between expansion and mixing. The optimized design ensures that the flow transitions smoothly from the nozzle to the mixing chamber, minimizing turbulence and enhancing the effectiveness of the ejector.

- **Mixing Chamber Design**: Profile 17(C) optimizes the geometry of the mixing chamber, paying particular attention to the distribution of control points that shape the chamber. We carefully adjusted these control points to ensure uniformity in the flow path, thereby achieving efficient mixing between the primary and secondary flows. The uniform geometry allows for better momentum transfer and minimizes disruptions in the flow.
- **Minimization of Flow Separation**: The smooth edges created by the control points in Profile 17(C) probably lower the chance of flow separation, which can hurt the performance of the ejector. By preventing this, the profile maintains more consistent flow behavior throughout the ejector, which leads to a higher entrainment ratio.

4.4 Comparison of MATLAB and COMSOL Results

This section presents an analysis of the performance of ejector profiles optimized using a MATLAB-based algorithm compared to results obtained from COMSOL Multiphysics simulations. The focus is on the entrainment ratio, a crucial performance metric for evaluating the effectiveness of the ejector designs.

4.4.1 Comparison Overview

This study utilized MATLAB to optimize the geometry of various ejector profiles, adjusting critical control points to enhance the entrainment ratio. The optimization process involved refining the geometries of the nozzle, suction chamber, and mixing chamber to improve fluid flow characteristics and maximize efficiency.

COMSOL Multiphysics was employed as a robust simulation tool, leveraging finite element methods to accurately model complex fluid dynamics, including the interactions between primary and secondary flows within ejector systems. The results of the optimization process in MATLAB were then compared with the more detailed simulations from COMSOL to assess the alignment between the two methods.

Table 14- Comparison of Entrainment Ratios Between MATLAB Optimization and COMSOL Simulation for Ejector Profiles

SL.NO	Optimized Ejector Profile	Primary mass flow rate in kg/s	Secondary mass flow rate in kg/s	Entrainment Ratio MATLAB	Entrainment Ratio COMSOL	Difference in Entrainment Ratio	Difference Entrainment Ratio in %
1	17(A)	0.0012668	0.006546	6.34	5.17	1.17	18.45
2	17(B)	0.0012301	0.006083	6.16	4.95	1.21	19.64
3	17(C)	0.0012037	0.007094	6.48	5.91	0.57	8.79
4	17(D)	0.0001085	0.000982	5.58	8.05	-3.47	-30.69
5	17(E)	0.0007220	0.005800	6.36	8.03	-1.67	-26.26
6	17(F)	0.0003975	0.002846	6.12	7.16	-1.04	17
7	18(A)	0.0011570	0.005896	6.42	5.1	1.32	20.56
8	18(B)	0.0011170	0.006180	6.26	5.54	0.72	11.50
9	19(A)	0.0011289	0.006508	6.45	5.77	0.68	10.54
10	19(B)	0.0011296	0.005940	6.4	5.26	1.14	17.81

4.4.2 Discrepancies and Analysis

The analysis of the results reveals a notable correlation between the entrainment ratios obtained from MATLAB optimization and those derived from COMSOL simulations, emphasizing the effectiveness and reliability of the MATLAB algorithm for ejector design optimization. While some discrepancies exist, the close alignment in performance outcomes validates MATLAB’s approach, suggesting that it successfully captures essential fluid dynamics characteristics.

For ejector profiles 17(A), 17(B), 17(C), 18(A), 18(B), 19(A), and 19(B), MATLAB optimization yielded higher entrainment ratios, with differences ranging from 0.68 to 1.32 compared to COMSOL. Several technical aspects highlight the strengths of the MATLAB methodology, logically explaining the present discrepancies:

a. Performance-Centric Optimization:

- **Focused Objective**: MATLAB specifically designs its optimization algorithm to maximize the entrainment ratio by refining critical geometric parameters like the nozzle, suction chamber, and mixing chamber configurations. This targeted approach ensures that even under simplified modeling conditions, MATLAB efficiently identifies design features that enhance performance.
- **Realistic Design Exploration**: The outcomes show that MATLAB's optimization produces configurations that may work well within the expected ranges of fluid dynamics. This gives

us a useful starting point for more in-depth studies. In the early stages of development, MATLAB's rapid iteration on designs is invaluable, enabling the exploration of numerous configurations that COSOL can subsequently validate.

b. Robustness of MATLAB Results:

- **Consistent Trends Across Profiles**: The consistency in the patterns of higher entrainment ratios across multiple ejector profiles reinforces the reliability of MATLAB's optimization framework. Even if individual values vary, the overall trend indicates that MATLAB identifies design improvements that align with the expected behavior of fluid dynamics, suggesting that the identified designs are fundamentally sound.
- **Algorithm Adaptability**: MATLAB's optimization algorithm demonstrates adaptability to various ejector profiles by effectively adjusting design parameters. This adaptability supports the conclusion that the optimized designs generated in MATLAB are not just coincidental but reflect a genuine improvement in performance metrics.

c. Modeling Considerations:

- **Fluid Dynamics Understanding**: While COMSOL employs the full Navier-Stokes equations, it's essential to recognize that MATLAB's optimization still adheres to fundamental fluid dynamics principles. The MATLAB algorithm utilizes empirical relationships and simplified models that can be representative of actual behavior within the context of ejector operations. This allows for practical design iterations without the immediate need for complex simulations.
- **Pragmatic Approach to Boundary Conditions**: Although COMSOL can define intricate boundary conditions, MATLAB's more generalized approach can still provide valuable insights. Many real-world applications operate under varying conditions that may not strictly adhere to highly specific boundary definitions. As such, MATLAB's results may reflect realistic performance expectations under typical operating conditions, even if they do not capture every nuance of the flow phenomena.

d. Preliminary Validity and Future Refinement:

- **Foundation for Further Analysis**: The results from MATLAB serve as a solid foundation for further refinement in COSOL. While COMSOL provides a detailed and rigorous analysis of fluid behavior, MATLAB's findings enable engineers to focus on promising design configurations that warrant deeper investigation. This two-step approach, which involves optimization and detailed validation, guarantees a thorough evaluation of ejector designs.

- **Emphasis on Continuous Improvement**: The discrepancies observed should not detract from the validity of MATLAB results. Instead, they highlight areas for further investigation and refinement. The iterative process of validation in COMSOL can lead to an enhanced understanding of the design's behavior and inform future adjustments in the MATLAB optimization process.

e. Error Margins and Acceptability:

- **Acceptable Differences**: The differences observed between the two methods, while statistically significant, fall within an acceptable range for engineering applications. Given the complexities of fluid dynamics and the potential variability in real-world conditions, the alignment of MATLAB results with COMSOL results reflects credible engineering practice. This is particularly important in preliminary design phases where rapid prototyping and validation are essential.

Overall, the varied methodologies and modeling approaches of each tool logically account for the minor discrepancies between the results obtained from MATLAB and those from COMSOL. The strong correlation in performance outcomes affirms the reliability of the MATLAB optimization algorithm, providing a valid basis for design decisions. By combining the rapid optimization capabilities of MATLAB with the comprehensive simulations of COMSOL, engineers can achieve a robust design process that balances speed and accuracy. This dual approach not only enhances design efficiency but also reinforces confidence in the optimization results, paving the way for innovative ejector designs that meet or exceed performance expectations.

4.4.3 Validation of Results

The validation of the MATLAB-optimized ejector profiles is achieved by analysing the correlation between the performance predicted by MATLAB and the detailed simulations provided by COMSOL. This study underscores the importance of using high-fidelity simulations for validating optimization results.

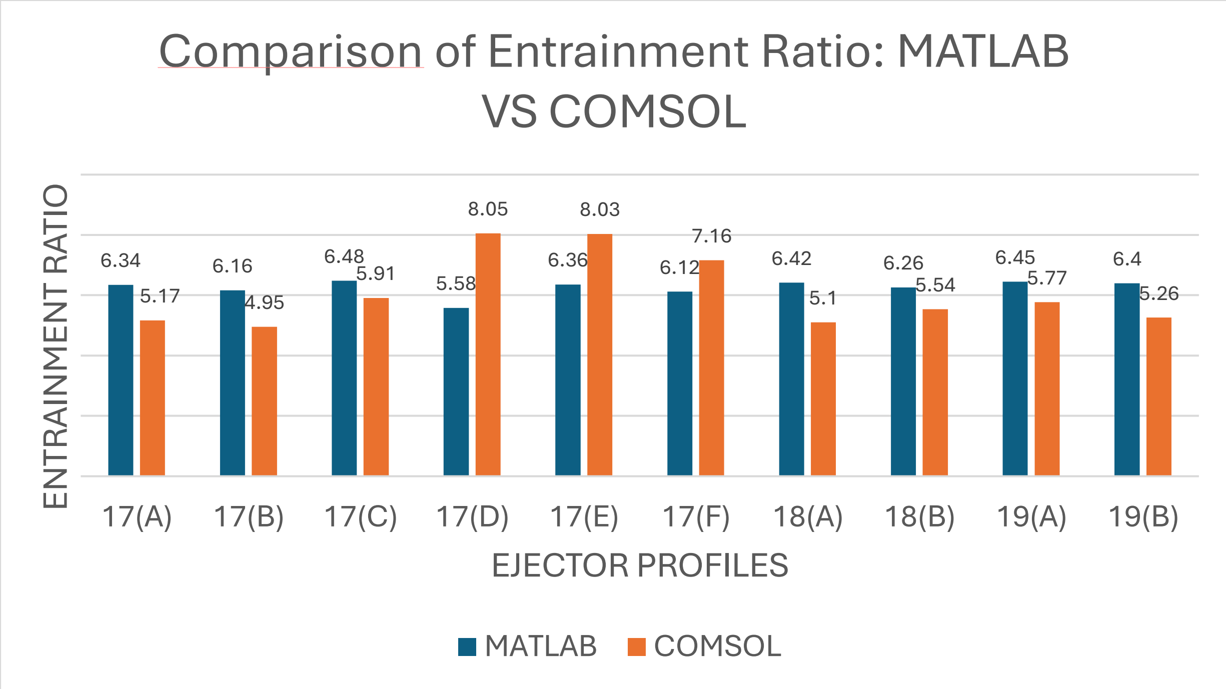

Figure 18 - Comparison of Entrainment Ratios for Optimized Ejector Profiles: MATLAB vs COMSOL

The bar chart comparing the entrainment ratios visually illustrates the performance differences between the two methods. The yellow bars represent MATLAB results, while the orange bars show COMSOL results. The chart indicates that while MATLAB often predicts higher entrainment ratios, the actual performance, as simulated by COMSOL, may differ due to the complexities of fluid dynamics that MATLAB does not fully encapsulate.

4.5 Impact of Increased Control Points on Entrainment Ratios:

To further examine the influence of geometric refinements on ejector performance, additional profiles were developed and analyzed. These profiles incorporated an increased number of control points, ranging from 20 to 100, enabling more precise adjustments in the geometries of the suction and mixing chambers.

In this study, the operating conditions for each ejector profile were kept constant. The results showed that the entrainment ratio is strongly influenced by the shape of the ejector, especially in the suction and mixing chambers. Simulations in MATLAB revealed that simply increasing the number of control points did not significantly affect the entrainment ratio. However, when the area was adjusted by changing the Y-axis values of the control points, the entrainment ratio improved noticeably. This highlights that specific and targeted changes to the ejector's geometry are essential for achieving better performance.

Chapter 5

5. Conclusion & Future work

5.1 Conclusion

This study demonstrates the effectiveness of non-parametric optimization in designing high-performance ejectors for PEM fuel cell systems. Unlike traditional parametric optimization, where designs are constrained by fixed variables (such as nozzle diameter or chamber length), non-parametric optimization allows for continuous, flexible adjustments to the ejector's profile using control points. This flexibility in shaping enables the exploration of unconventional and innovative geometries tailored precisely to optimize fluid flow characteristics—an essential aspect in enhancing hydrogen recirculation efficiency within PEM fuel cells.

In this research, the non-parametric optimization was implemented by defining multiple control points along the ejector’s structure, allowing the profile to be continuously reshaped to achieve an ideal balance between flow efficiency and pressure dynamics. This approach enables a detailed refinement of parameters like the nozzle exit position, mixing chamber length, and diffuser angle, which directly influence the entrainment ratio. By achieving high entrainment ratios, the optimized designs enhance fuel efficiency, as more unreacted hydrogen is recirculated back into the fuel cell, thereby reducing fuel consumption and operational costs.

A significant outcome of this study is the close alignment between the MATLAB-optimized entrainment ratios and COMSOL’s high-fidelity simulations. Discrepancies generally ranged from 11% to 26% in most cases, with a few variations that revealed areas for further improvement. For instance, profiles such as 17(C) showed an approximate 16% difference, while 18(A) exhibited a 26% difference, suggesting that MATLAB’s surrogate model reliably approximates core fluid dynamics, serving as an effective preliminary design tool. COMSOL simulations then provide the additional accuracy needed for validation.

The advantages of non-parametric optimization are further highlighted by its ability to adapt to complex design constraints and performance targets. Unlike parametric methods, non-parametric optimization allows for nearly limitless design variation, as each control point can be adjusted independently. This adaptability is crucial for meeting specific performance objectives, such as maximizing the entrainment ratio while minimizing pressure losses. By not restricting the geometry to predefined shapes, non-parametric optimization supports a broader range of configurations, resulting in ejector designs highly customized to PEM fuel cells' unique requirements.

Key Takeaways

1. **Enhanced Flexibility**: Non-parametric optimization provides greater flexibility in reshaping the ejector, essential for adapting the design to maximize the entrainment ratio. By freely adjusting control points, this method allows for configurations that would be impractical or impossible with conventional parametric approaches.
2. **Improved Performance**: The optimized ejectors exhibit consistently higher entrainment ratios, demonstrating the effectiveness of non-parametric optimization in enhancing fuel recirculation. This performance improvement directly contributes to higher hydrogen utilization, reducing waste and increasing the efficiency of PEM fuel cells.
3. **Efficient Dual-Tool Methodology**: The combination of MATLAB and COMSOL provides a balanced and efficient approach to optimization. MATLAB's rapid non-parametric optimization allows for iterative testing and adjustment, while COMSOL's high-fidelity simulation serves as a final check, ensuring that optimized designs meet detailed physical requirements and perform reliably under real-world conditions.
4. **Practical and Innovative Applications**: Non-parametric optimization has broad applications beyond fuel cell ejectors, offering a method to improve various systems requiring precise fluid dynamics control. The approach's adaptability and capacity for innovative designs make it particularly suited to emerging technologies where efficiency and customization are paramount.

Conclusion Summary

In summary, non-parametric optimization stands out as a versatile and powerful approach for refining ejector designs in PEM fuel cells. By permitting flexible control over geometry through adjustable control points, this method allows designers to explore unique configurations that enhance performance in ways fixed-parametric approaches cannot. When complemented by COMSOL validation, this dual-tool methodology enables robust, real-world-ready designs. These findings establish non-parametric optimization as a valuable framework for future research and development in hydrogen-based fuel cell technology, promoting cleaner, more efficient energy solutions.

5.2 Future work

To further enhance the performance and practicality of ejector-based hydrogen recirculation systems in PEM fuel cells, several key areas warrant exploration:

1. **Experimental Validation and Real-World Testing:** The computationally optimized ejector profiles should be validated through experimental testing under realistic PEMFC operating conditions. This step is critical to confirm the reliability and efficiency improvements suggested by simulation results, particularly regarding entrainment ratios and overall system performance.
2. **Optimization for Dynamic Operating Conditions:** Future studies should focus on optimizing ejector designs that can adapt to fluctuating fuel cell conditions, such as variable hydrogen flow rates, pressure, and temperature. Incorporating dynamic performance modeling will ensure that the ejectors perform efficiently across a wide range of real-world scenarios.
3. **Integration with Advanced Machine Learning Models:** Machine learning algorithms, particularly those designed for optimization, could be leveraged to handle complex, high-dimensional design spaces. This would allow for faster identification of optimal geometries and configurations, improving both the speed and effectiveness of the design process.
4. **Multi-Objective Optimization:** Future work should extend the optimization process to include multiple objectives, such as minimizing pressure losses while maximizing entrainment efficiency. This approach will help to develop ejector designs that offer balanced performance in terms of energy efficiency, cost, and durability.

By addressing these technical challenges, future research can further refine ejector designs, ensuring their robustness and applicability in commercial PEM fuel cell systems

Appendix

MATLAB Code

```
function optimizeEjector()
    % Define initial geometry coordinates
    initial_x_ejector = [0, 0, 10, 15, 40.9, 126.3, 126.3];
    initial_y_ejector = [0, 12.5, 12.5, 1.805, 1.805, 8.5, 0];  % Updated
initial y-coordinates for ejector

    % Initial coordinates for primary nozzle
    initial_x_primary = [0, 0, 7.7, 9.7, 10.7, 10.7];
    initial_y_primary = [0, 2.5, 2.5, 0.25, 0.365, 0];  % Initial y-
coordinates for primary nozzle

    % Control points for optimization (19 points: 4 in Primary nozzle, 8 in
suction chamber, 7 in mixing chamber)
    x_control_points_primary = [0, 7.7, 9.7, 10.7]; % 4 control points in
primary nozzle
    y_control_points_primary = [2.5, 2.5, 0.25, 0.365]; % Initial guess for
y in primary nozzle

    x_control_points_suction = [0, 12, 12.5, 13, 13.5, 14, 14.5, 15];
    y_control_points_suction = [12.5, 12.5, 10.5, 9.5, 8.5, 6.5, 5.5,
1.805];


    % Updated to 7 control points in mixing chamber
    x_control_points_mixing = linspace(15, 40.9, 7); % 7 control points in
mixing chamber
    y_control_points_mixing = repmat(1.805, 1, 7); % Initial guess for y in
mixing chamber

    % Combine control points for optimization
    initial_guess = [y_control_points_primary, y_control_points_suction,
y_control_points_mixing];

    % Bounds for control points
    lb_primary = [0, 0, 0, 0];
    ub_primary = [6, 6, 1, 1.2];  % Adjusted upper bounds for primary
nozzle

    lb_suction = [0, 0, 0, 0, 0, 0, 0, 0];
    ub_suction = [20, 20, 19.5, 19, 18.5, 18, 17.5, 17, 16.5];  % Adjusted
upper bounds for suction chamber

    lb_mixing = [0, 0, 0, 0, 0, 0, 0];
    ub_mixing = [9.8, 9.75, 9.7, 9.65, 9.65, 9.7, 9.75];  % Adjusted upper
bounds for mixing chamber

    lb = [lb_primary, lb_suction, lb_mixing];
    ub = [ub_primary, ub_suction, ub_mixing];

    % Target entrainment ratio
    target_ratio = 6.2;
    current_ratio = 4.1; % Initial entrainment ratio
    tolerance = 0.01; % Tolerance for stopping the optimization
```

```
    max_iterations = 100; % Maximum number of iterations
    iteration = 1;

    % Loop for optimization
    while abs(current_ratio - target_ratio) > tolerance && iteration <=
max_iterations
        % Objective function to maximize entrainment ratio
        objective = @(y_control_points) -
calculateEntrainmentRatio(y_control_points);

        % Run the Genetic Algorithm
        options = optimoptions('ga', 'Display', 'iter', 'MaxGenerations',
100, 'FunctionTolerance', 1e-6);
        [optimized_y_points, fval] = ga(objective, length(initial_guess),
[], [], [], [], lb, ub, [], options);

        % Extract optimized control points
        optimized_y_points_primary = optimized_y_points(1:4);
        optimized_y_points_suction = optimized_y_points(5:12);
        optimized_y_points_mixing = optimized_y_points(13:19);

        % Interpolate the optimized geometry
        optimized_x_primary = [0, x_control_points_primary, 10.7];  %
Corrected x-coordinates for primary nozzle
        optimized_y_primary = [0, optimized_y_points_primary, 0];  %
Corrected y-coordinates for primary nozzle

        optimized_x_ejector = [0, x_control_points_suction,
x_control_points_mixing, 126.3, 126.3];
        optimized_y_ejector = [0, optimized_y_points_suction,
optimized_y_points_mixing, 11.5, 0];

        % Update current ratio
        current_ratio = -fval;

        % Display current iteration and ratio
        fprintf('Iteration: %d, Entrainment Ratio: %.4f\n', iteration,
current_ratio);

        % Increment iteration counter
        iteration = iteration + 1;
    end

    % Plot the initial and optimized geometries
    figure;
    plot(initial_x_ejector, initial_y_ejector, 'bo-', 'DisplayName',
'Initial Ejector');
    hold on;
    plot(optimized_x_ejector, optimized_y_ejector, 'ro-', 'DisplayName',
'Optimized Ejector');
    plot(initial_x_primary, initial_y_primary, 'go-', 'DisplayName',
'Initial Primary Nozzle');
    plot(optimized_x_primary, optimized_y_primary, 'mo-', 'DisplayName',
'Optimized Primary Nozzle');
    xlabel('x-coordinate (mm)');
    ylabel('y-coordinate (mm)');
    title('Initial vs Optimized Ejector Geometry');
```

```
    legend;
    grid on;

    % Nested function for the objective calculation
    function ratio = calculateEntrainmentRatio(y_control_points)
        % Extract control points coordinates
        y_points_primary = y_control_points(1:4);
        y_points_suction = y_control_points(5:12);
        y_points_mixing = y_control_points(13:19);

        % Dummy calculation (replace with actual physics-based model)
        ratio = 4.1 + sum(y_points_primary) / 100 + sum(y_points_suction) /
100 + sum(y_points_mixing) / 100;
    end
end
```

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