MODELING AND ADJOINT OPTIMIZATION OF HEAT EXCHANGER GEOMETRIES

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OF HEAT EXCHANGER GEOMETRIES

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OF HEAT EXCHANGER GEOMETRIES

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For my mother, father, brother, sister, and niece

SUMMARY

In today's society, with an increasing need for energy worldwide and at the same time a growing awareness of its negative consequences, optimizing and reducing energy consumption has become important for sustainability. The process of optimizing the appliances in large industry and household scale contributes to the minimization of the global energy consumption. In order to increase the efficiency of these appliances, various optimizations are employed, such as the shape optimization.

In this thesis, a shape optimization method is used to modify the geometry of an existing heat exchanger. The heat exchanger is used in a domestic boiler and the shape optimization is a crucial step for its fast development. Currently, the shape of the heat exchanger is highly dependent on its manufacturing process. Thus, more complex shapes are investigated and their effects on the heat transfer and pressure drop are evaluated in this thesis. Two aspects need to be investigated for this heat exchanger optimization: the complex internal flow within the heat exchanger, and the performance of the optimization method as well as its resulting shapes. Since the heat exchanger consists of different flow regimes due to its complex geometry, a detailed study on these regimes is conducted prior to the optimization procedure. Furthermore, the complex geometry of this heat exchanger leads to different models used in this thesis. Therefore this thesis is divided into three parts based on the models: the three-dimensional single cylinder, the two-dimensional cylinder arrays, and the three-dimensional cylinder array.

In optimizing the heat exchanger, the shape optimization method is justified as the most suitable method. Using the ANSYS Fluent's adjoint shape optimization method, the pressure drop and the heat transfer of the heat exchanger are optimized. This method has been used in the past for optimizing various geometries, yet to the author's knowledge, no detailed study on the cylinder array has been published. Consequently, a study on the adjoint parameters and its effect on the overall performance of the optimization procedure is of importance.

To investigate these aspects, three sets of studies are conducted, and are presented in the three parts of the thesis. Firstly, an unsteady Direct Numerical Simulation (DNS) of a three-dimensional single cylinder in a cross-flow is performed at critical Reynolds number, $Re_D = 2000$. This flow is categorized as a transition flow in shear layer regime, a regime that is not widely studied in literature aside from detailed numerical simulations at $Re_D = 3300$ and $Re_D = 3900$. The findings of this work provide an insight into the heat transfer over a circular

cylinder in a transitional flow. Due to the periodic flow and the three-dimensional motions at this Reynolds regime, further studies using the single cylinder domain are conducted at lower Reynolds number, $Re_D = 10$. At this flow regime, a steady adjoint shape optimization procedure is performed with a conjugate heat transfer model. The optimization results produce the optimized shape of a single cylinder as well as a reduction of the drag force and an improvement of the heat transfer.

The second part of the thesis consists of two-dimensional studies of cylinders in an array. A few studies on the shape optimization of cylinder array have been presented in literature, however none of these studies employ the adjoint method. In this part of the thesis, four topics are elaborated: the first deals with detailed single-objective and multi-objective optimization cases where pressure drop and heat transfer are chosen to be the objectives. The results of these cases provide insight into the correlation between the heat transfer and the pressure drop of an array of cylinders for this specific flow. Second, both circular and elliptical cylinders are modeled and optimized. The final optimized shapes of both cases are compared and their performances are visualized in the so-called *objective space* in terms of heat transfer and pressure drop. This study yields an overview of the objective space and the possible optimization paths for these cases. Third, various adjoint parameters are studied and its effects on the final optimized geometries are shown. Finally, the challenges that arise when applying the ANSYS adjoint automatic shape optimization procedure are explained and the solutions are presented.

In the last part of the thesis, a three-dimensional array of cylinders is modeled. A more complex boundary condition is used, namely the periodic boundaries at the inlet and at the outlet of the domain. The conjugate heat transfer model is employed and the domain is optimized for a flow at $Re_D = 100$. The optimization results show that the adjoint optimization procedure cannot successfully produce a shape that yield improvements in both objectives, alternately optimizing only for one objective. Following this, the investigation of the failure of the adjoint optimization procedure is presented. Studies on the weight factors and optimizer performance are conducted and the results are compared with that of the successful optimized single cylinder case. Possible cause of the failure of the adjoint optimization procedure is presented as well as the best practice and recommendations for future work.

SAMENVATTING

In onze hedendaagse maatschappij, met wereldwijd een oplopende behoefte aan energie en tegelijkertijd een groeiend besef van de negatieve consequenties hiervan, is het optimaliseren en terugdringen van energieverbruik een belangrijk thema. Er vallen op dit gebied nog winsten te behalen bij zowel industriële als huishoudelijke apparaten. Verschillende optimalisatiemethoden zijn beschikbaar om bij deze apparaten een efficiëntieslag te slaan, zoals de vormoptimalisatiemethode.

In dit proefschrift wordt de vormoptimalisatiemethode gebruikt om de bestaande geometrie van een warmtewisselaar te wijzigen, die gebruik wordt in een huishoudelijke verwarmingsketel. Momenteel is de vorm van de warmtewisselaar sterk afhankelijk van het productieproces. Aldus worden meer complexe vormen onderzocht en hun effecten op de warmteoverdracht en drukval worden in dit proefschrift geëvalueerd. Twee aspecten worden onderzocht: de complexe interne stroom in de warmtewisselaar, en de prestaties van de optimalisatiemethode evenals de resulterende vormen. Omdat de warmtewisselaar vanwege zijn complexe geometrie uit verschillende stromingsregimes bestaat, wordt voorafgaand aan de optimalisatieprocedure een gedetailleerd onderzoek naar deze regimes uitgevoerd. Bovendien leidt de complexe geometrie van deze warmtewisselaar tot verschillende modellen die in dit proefschrift worden gebruikt. Dit proefschrift is daarom verdeeld in drie delen op basis van de modellen: de driedimensionale enkele cilinder, de tweedimensionale rij van cilinders en de driedimensionale rij van cilinders.

Bij het optimaliseren van de warmtewisselaar wordt de vormoptimalisatiemethode gekozen als de meest geschikte methode en de rechtvaardiging wordt in dit proefschrift uitgelegd. Met behulp van de *adjoint* vormoptimalisatiemethode van ANSYS Fluent worden de drukval en de warmteoverdracht van de warmtewisselaar geoptimaliseerd. Deze methode is in het verleden gebruikt om verschillende geometrieën te optimaliseren. Voor zover de auteur weet, is er echter geen gedetailleerde studie over de rij van cilinders gepubliceerd. Bijgevolg is het onderzoek naar de *adjoint* parameters en het effect ervan op de algehele prestaties van de optimalisatieprocedure van belang.

Om deze aspecten te onderzoeken, worden drie sets studies uitgevoerd en gepresenteerd in de drie delen van het proefschrift. Ten eerste wordt een Directe Numerieke Simulatie (DNS) van een dwars aangestroomde cilinder uitgevoerd op een kritisch Reynolds getal van $Re_D = 2000$. Deze stroming is gecategoriseerd als een transitie in het *shear layer* regime, een regime dat niet uitgebreid is bestudeerd in

de literatuur, afgezien van de gedetailleerde numerieke simulaties bij $Re_D = 3300$ en $Re_D = 3900$. De bevindingen van dit werk geven inzicht in de warmteoverdracht van een cirkelvormige cilinder in een transitiegebied. Vanwege de periodieke strooming en de driedimensionale bewegingen bij dit Reynolds-regime, worden verdere onderzoeken van het enkele cilinderdomein uitgevoerd voor een lager Reynolds getal, $Re_D = 10$. Bij dit stroomingsregime wordt een geconjugerd warmteoverdrachtsmodel van de enkele cilinder in een uniforme strooming ontwikkeld. De optimalisatieresultaten tonen de geoptimaliseerde vorm van een enkele cilinder, evenals een vermindering van de stromingsweerstand en een toename van de warmteoverdracht.

Het tweede deel van het proefschrift bestaat uit tweedimensionale studies van cilinders in een rij. In de literatuur is weinig onderzoek gedaan naar vormoptimalisatie van een rij van cilinders, en geen van deze onderzoeken maakt gebruik van de adjoint methode. In dit deel van het proefschrift worden vier onderwerpen uitgewerkt: allereerst worden er een aantal gevallen gepresenteerd van gedetailleerde *single-objective* en *multi-objective* optimalisaties met warmteoverdracht en drukval als de te optimaliseren parameters. De resultaten van deze gevallen geven inzicht in de correlatie tussen de warmteoverdracht en de drukval van een rij van cilinders voor deze specifieke strooming. Ten tweede worden zowel ronde cilinders als elliptische cilinders gemodelleerd en geoptimaliseerd. De uiteindelijke geoptimaliseerde vormen van beide gevallen worden vergeleken en de prestaties ervan worden afgebeeld in de zogenaamde *objective space* in termen van warmteoverdracht en drukval. Deze studie geeft een overzicht van de *objective space* en de mogelijke optimalisatiepaden voor deze gevallen. Ten derde worden verschillende adjoint parameters en de effecten ervan op de uiteindelijke geoptimaliseerde geometrieën bestudeerd. Ten slotte worden de uitdagingen die zich voordoen bij het toepassen van de ANSYS adjoint automatische vormoptimalisatieprocedure uitgelegd en worden de oplossingen gepresenteerd.

In het laatste deel van het proefschrift wordt een driedimensionale rij van cilinders gemodelleerd. Een meer complexe randvoorwaarde wordt gebruikt, namelijk de periodieke randvoorwaarde aan de inlaat en aan de uitlaat van het domein. Het conjugate warmteoverdrachtsmodel wordt gebruikt en het domein is geoptimaliseerd voor een strooming met $Re_D = 100$. Met dit model is gebleken dat de adjoint optimalisatieprocedure niet met succes een vorm kan produceren die beide objectieven verbetert, echter slechts één van beide. In dit deel van het proefschrift wordt het onderzoek naar het falen van de adjoint optimalisatieprocedure gepresenteerd. Studies naar de gewichtsfactoren en de prestatie van de optimalisatiemethode worden uitgevoerd en de resultaten worden vergeleken met die van de succesvol geoptimaliseerde enkele cilinder. Een mogelijke oorzaak van het mislukken van de adjoint optimalisatie-

procedure wordt gepresenteerd, evenals verschillende *best practices* en aanbevelingen voor toekomstig onderzoek.

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Part I

FUNDAMENTALS

In this part, introduction to the problem as well as theoretical background are presented.

INTRODUCTION

Heat exchangers have been widely used in many industrial applications to transfer heat between two or more fluids. The use of heat exchangers in industrial processes triggers studies for the development of heat exchangers in terms of efficiency and cost. The production of energy-efficient heat exchangers will contribute to the reduction of the world energy consumption. To save energy, one example case is by performing an optimization process of the heat exchanger used for a domestic boiler.

A domestic boiler is used to heat water to supply a central heating system, or hot water for taps, or both. In this thesis, the 'boiler' specifically refers to an existing gas-fuelled domestic boiler produced by Bosch Thermotechnology. In optimizing the Bosch boiler, the main objective is to reduce the cost while obtaining the best possible performance of the appliance. To increase the performance of such appliance, various efforts have been carried out in the field of heat exchanger optimization. Heat transfer enhancement, reduction of pressure drop, emission, and material volume are some examples of the optimization goals. Some parameters of interest that affect the optimization goals will be discussed in this thesis, such as: heat transfer, pressure drop, and drag force. To achieve these goals, modification of the existing appliance is commonly carried out. Adding physical structure such as winglets and fins can manipulate the flow by introducing vortex-induced flow or enhance the heat transfer. Another way of increasing the heat transfer is by adding heat-enhanced particles to the flow field. In this thesis, no physical structure is added, nor the fluid is changed. This work focuses on the design process by altering the geometry of the current heat exchanger.

In performing the optimization of the Bosch boiler, a simulation-based approach is used in this thesis. A simulation-based approach can greatly reduce the time needed to arrive at a candidate design when compared to non-simulation based methods [1]. Hence, modeling of the current heat exchanger is of importance in the workflow of the current optimization process. Furthermore, the utilization of a specific optimization method namely the adjoint method will be discussed in more detail in this thesis.

The background and problem definition will be explained in Chapter 1.1. Subsequently, an introduction to the heat exchanger optimization will be given in Chapter 1.2. Chapter 1.3 explains shortly about the flow around cylinders and its significance in the current boiler application. The main objective of this research is presented in Chapter 1.4. Finally, Chapter 1.5 explains the outline of the thesis.

Figure 1.1: (a) Wall-mounted Bosch boiler for domestic heating and hot water supply. The water channel is visible as the rectangular slots vertically lined up on the outer side of the main compartment. (b) Three-dimensional model of the boiler. The spiraling water channel is seen on the outside wall of the boiler. (c) Cross-section of the boiler, cut on its symmetry plane. Note that the boiler is not rotationally axisymmetric, but 180° symmetric.

1.1 BACKGROUND

The Bosch boiler is depicted in Figure 1.1. This wall-mounted boiler is used to supply hot water for the central heating system and the hot water tap, with a capacity of 3-24 kW. At the top of the boiler, the burner for the gas combustion is located. The hot exhaust gas flows in the inner chamber towards the bottom of the boiler, thus transferring heat to the cold water through the heat exchanger. In the center of the hot chamber, a cylindrical baffle is placed to regulate the flow of the hot gas. The cold water flows in the outer channels of the heat exchanger in a spiralling manner (Figure 1.1b).

The heat exchanger is the pin-fin type, with various shapes of the fin and pins along the streamwise direction of the exhaust gas. The upstream part of the heat exchanger consists of one row of fins. The middle part of the heat exchanger consists of three rows of circular cylinders, while the bottom part consists of multiple rows of D-shaped cylinders with the round part of the D-shape located upstream. The straight part of the D-shape is used to increase turbulence at the back of the cylinder. Note that the heat exchanger is not rotationally axisymmetric, but half-symmetric (Figure 1.1c). The cylindrical pins are made by sand casting process, thus adding a limitation for the current optimization process. However, for the sake of computational evaluation, this limitation is not considered in the current thesis and is left for future work and improvement.

Due to the various fins and pin encountered by the gas flow along the streamwise direction, various flow patterns could result due to the interaction between the fluid and the different shapes of the fins and pins. As the hot gas is cooled towards the outlet, various Reynolds numbers also develop within the heat exchanger: low Reynolds flow (Re_D in the order of 10^2) at the top part and high Reynolds flow at the bottom ($Re_D \sim 1000 - 2000$). This adds complexity for the modeling of the heat exchanger, especially the different flow regimes for the different parts of the heat exchanger. Moreover, the transitional flow occurs in the range of Reynolds number that is not much studied numerically ($Re_D = 1000 - 2000$). To study this heat exchanger, this thesis is focused on two subjects: the numerical study of the flow at the transition regime, and the adjoint shape optimization to optimize the heat exchanger.

1.2 HEAT EXCHANGER OPTIMIZATION

The aim of this work is to find an improved design of the current heat exchanger in terms of heat transfer and the reduction of pressure drop or drag force. Some general techniques for heat transfer enhancement can be achieved by two types of methods: active and passive [2]. Passive enhancement involves processes that require no external power, while active enhancement needs external power. Examples of passive techniques are the utilization of special surface geometries and fluid additives. For the active technique, other means of external power can be employed, such as the electromagnetic field. In this thesis, a passive heat transfer enhancement technique is studied for the gas-side heat transfer. The current gas-side heat transfer surface of the pins will be modified using the adjoint shape optimization procedure to obtain a new optimized surface.

The modification of the pin surface will affect not only the heat transfer of the system, but also the pressure drop and surface drag force. Generally, to enhance the heat transfer, one will enlarge the heat transfer surface area. However, for a confined flow in a channel, this results in a higher pressure drop of the system. Thus, increasing the performance of the heat exchanger possess its own challenges since heat transfer and pressure drop are two contradicting objectives. Therefore, the relation between heat transfer and pressure drop for this specific system will be studied in this research.

1.3 FLOW AROUND CYLINDERS

As previously mentioned, the current heat exchanger consists of different shapes of fin and pin and the main objective of this study is to find new shapes with better performance. However, to simplify the numerical model and to find literature about already studied shapes,

the circular cylinder is deemed to be a good starting point. Various research in the field of flow around cylinder have been conducted in the past. Additionally, some works about flow around circular cylinder in transitional regime have been carried out, although mostly are not in the same regime as the current heat exchanger. Nevertheless, the abundant information in the field of flow around cylinders are essential for conducting this study. Therefore, a brief introduction to the flow around cylinders will be explained in this subchapter.

Different shapes of cylinder have been used in heat exchangers to increase the heat transfer area. Circular cylinders, elliptical cylinders, and square cylinders are the most common shapes. Some works studying the flow around circular, elliptical, and square cylinders are [3, 4, 5]. In terms of aerodynamic study, drop-shaped cylinders can also be employed for heat exchangers [6] with the advantage of its low pressure drop. Considering the current D-shape of the cylinder, a simplification is made to select the shape of the numerical domain. Circular and elliptical cylinders are used in this thesis. The flow around a circular cylinder and an elliptical cylinder will be discussed in the following passage.

Flow around a circular cylinder has been a topic of extensive research since the 18th century. Different flow behaviors were observed on the disturbed flow and the effect of parameters such as flow velocity, cylinder size, fluid density and viscosity were studied. The disturbed flow is characterized by a dimensionless parameter called Reynolds number $Re_D = \frac{\rho u D}{\mu}$, which represents the ratio of inertial to viscous forces. Zdravkovich [7] divided the flow past a cylinder into five regimes based on the Reynolds number, ranging from fully laminar flow to fully turbulent flow, with three different regimes of transitional flow in between. The fully laminar state consists of three basic flow regimes: creeping flow, steady separation flow, and periodic laminar regime which range from $Re = 0$ up to approximately $Re = 180$. In these regimes, the flow is characterized by mostly two-dimensional motion perpendicular to the cylinder axis. The creeping flow exists for Reynolds number smaller than 5. The steady laminar regime is characterized by non-periodic flow at $Re_D = 5 - 30$. At $Re \sim 30 - 48$, the first instability occurs, marked by the existence of von Kármán vortex shedding.

At $Re > 180$, the first transition regime occurs. A so-called transition-in-wake state of flow is defined by the unstable three-dimensional flow further downstream in the far wake. The instability mode of eddy formation is shown by the turbulent eddy roll up, thus changing the shedding mode from laminar flow to a more irregular flow downstream. This change is defined by the sudden drop in shedding frequency f , formulated by the dimensionless Strouhal number, $St = \frac{fD}{u}$.

The second transition regime occurs between approximately $Re = 350$ to $Re = 2 \times 10^5$. In this regime, the transition occurs in the free

shear layer, a region close to the cylinder where the boundary layers continue to develop downstream. The onset of turbulence occurs in these layers, hence affecting the length and width of the near-wake flow. The transitional flow starts around $Re = 350$, marked by the oscillating motion of the free shear layers. With higher Re , discrete eddies start to appear from the rolled-up oscillating free shear layers and then finally burst into turbulent eddies. The transition from the oscillating free shear layer into discrete eddies is not clearly defined, as it ranges from $Re = 1000$ to $Re = 2000$ [7]. At Re approximately 2×10^4 to 4×10^4 , the turbulent eddies start to appear and intensify with higher Re up to 2×10^5 , where a sudden drop of the drag coefficient and jump of shedding frequency designate the third transition regime, namely the boundary layer transition regime.

The three-dimensional turbulent flow that forms at the boundary layers causes the delay of eddy formation. Further increase of Reynolds number changes the flow pattern from an asymmetric single-bubble regime into a symmetric two-bubble regime, then finally to the supercritical regime where all the periodicity of the flow disappears. Thus, this marks the onset of the fully turbulent flow at about $Re = 3.5 \times 10^6$ up to higher Re .

The study of flow around a circular cylinder has been extensive, however the real-life application of cylinders in heat exchangers mostly involves multiple cylinders arranged in an array. Generally, cylinder arrays can be categorized into two groups: in-line and staggered arrangement. Hence, study of flow around an array of cylinders is of importance. It is known that two cylinders in tandem could lead to interference effects, such as change in flow patterns, magnitude of forces, and eddy shedding [8]. Furthermore, cylinders are usually arranged in close spacing in a confined space, leading to the need to study interstitial flow. A more complex condition is for example, flow variation in space and time within the cylinder array due to the turbulence that is generated row after row [8]. Thus, for the current heat exchanger, it is difficult to find literature for a specific arrangement of cylinders operating at a specific condition of the fluid flow.

Similarly to a circular cylinder, an elliptical cylinder is also commonly employed in industrial application. However, unlike the circular cylinder, only limited information is available for the flow over an elliptical cylinder, even in the steady flow regime [4]. This is due to the numerous variations of the ellipse major and minor axis, which makes it difficult to categorize the flow regime. Some examples of the previous works are that of Dennis and Young [9] who studied the steady two-dimensional flow around an elliptical cylinder with aspect ratio $E = 5$ for different Reynolds number ($1 \leq Re \leq 40$). They also studied the effect of various angle of incidence ($0 - 90^\circ$) to the flow. Further study to differentiate flow regime was performed by Johnson et al. [10] who observed the

Table 1.1: List of used constant properties.

Material Property	Unit	Flue Gas	Solid
Density	$[kg/m^3]$	1	2650
Specific heat capacity	$[J/kgK]$	1006.43	910
Thermal conductivity	$[W/mK]$	0.0242	170
Viscosity	$[kg/ms]$	1.7894×10^{-5}	-

effect of various Reynolds numbers and aspect ratios to the onset of vortex shedding. In general, the steady regime was reported to end at Re 35 – 40, comparable to that of the commonly known value for circular and square cylinder at $Re_D = 40 - 45$ [4].

Since the heat exchanger in the present study lies in various ranges of Reynolds number, as well as different configurations and fluid properties, the discussion of the ellipse array application for the current heat exchanger will be presented in more details in Chapter 6. It should be noted that for both arrays of circular and elliptical cylinders, the drop in temperature along the streamwise direction affects the numerical simulation solution.

To numerically model the current heat exchanger, it is important to incorporate the effect of temperature on the fluid properties. Not only the gas properties, but the solid and water properties needs to be modeled as well. However, due to the limitations of the ANSYS Fluent adjoint add-on for a temperature-dependent material in a conjugate heat transfer case, constant properties are used throughout this thesis. This decision is made based on the justification that for each chapter in this thesis, only a part of the heat exchanger is modeled for a specific Reynolds number, rather than modeling the entire channel of the flue gas flow. Furthermore, it is computationally expensive to incorporate all the features of the real heat exchanger into the computational model, such as the solid-fluid heat transfer model, various Reynolds number flow (an unsteady direct numerical simulation is needed in this case), as well as performing the adjoint shape optimization procedure for the whole channel. Therefore, the results presented in Chapter 3-7 are restricted only for a specific short part of the heat exchanger and are based on the constant properties of the gas and the solid body.

The material properties for the current numerical model are based on the present heat exchanger properties and are listed in Table 1.1. The solid body of the pin is made of aluminium alloy AC 43000 AlSi10Mg.

1.4 RESEARCH OBJECTIVES

The following research questions are to be answered:

1. How significant are the differences between the two-dimensional and three-dimensional simulation results for the relatively low transitional fluid regime ($Re_D = 2000$) in terms of heat transfer and flow?
2. Is there a cross-sectional shape of the pin aside from the circular, elliptical, square, D-shaped, drop-shaped, and other known shapes that can result in a better heat transfer and pressure drop of the current system? If so, can this shape be obtained using the ANSYS Fluent adjoint method?
3. How does the cross-sectional shape of the pin look like if a three-dimensional shape optimization is to be performed to the pin with conjugate heat transfer?
4. How much does the pressure drop degrade when a single objective optimization is performed to improve the heat transfer, and vice versa?
5. What are the parameters in the ANSYS Fluent adjoint optimization procedure that can affect the resulting optimized shapes?

The first research question will be answered in Chapter 3. The second question will be answered throughout this thesis from Chapter 4-7. The third question is specifically answered in Chapter 4 and 7. The fourth question is answered in Chapter 5, while the last question is answered in Chapter 6.

1.5 OUTLINE OF THE THESIS

The main content of this thesis is divided into three parts. Part I consists of Introduction (Chapter 1) and Theoretical Framework (Chapter 2). Part II presents the results of three-dimensional simulations for a single circular cylinder. This part consists of Chapter 3 and Chapter 4. Part III shows the results of the two-dimensional simulation of cylinder arrays, and consists of Chapter 5 and Chapter 6. Finally, Part IV (Chapter 7) presents a study case of a three-dimensional simulation for the cylinder arrays.

For the general optimization theory and methodology, the readers are referred to Chapter 2. However, a more specific detail of the different methodologies used in each chapter of this thesis will be explained in the methodology section of the respective chapter. In Chapter 3, the results of the direct numerical simulation of flow and heat transfer over a circular cylinder at $Re_D = 2000$ will be presented. This flow regime represents the high Reynolds flow at the bottom of the Bosch heat exchanger. In this chapter, no adjoint shape optimization is performed. In Chapter 4, the first study case of the adjoint optimization is

introduced for a single circular cylinder with conjugate heat transfer in a low Reynolds flow regime, $Re_D = 10$. This flow regime represents the top part of the Bosch heat exchanger. Since a single cylinder is modeled, the selection of low Reynolds number is deemed necessary to avoid the first instability of the von Kármán vortex shedding while performing the adjoint optimization procedure. From the findings in this chapter, a more detailed study is presented in Chapter 5 for the two-dimensional adjoint optimization of the cylinder arrays. Both single and multi-objective optimization are explained in this chapter. Chapter 6 also discusses about the two-dimensional adjoint optimization of the cylinder arrays in more details. The difference between Chapter 5 and Chapter 6 lies in the (1) optimization procedure, where in Chapter 6 both parametric optimization and adjoint shape optimization are performed, (2) geometries of the initial domain, where Chapter 6 uses an ellipse domain aside from the circular cylinder domain, and (3) more adjoint parameters analysis are presented in Chapter 6. In Chapter 7, a three-dimensional adjoint optimization case is discussed for the staggered array with periodic boundary conditions. Finally, Chapter 8 presents the conclusion and remarks.

It should be noted that the works explained in this thesis regarding 'optimization' refers to the multi-objective shape optimization using the adjoint method, unless stated otherwise. Furthermore, this thesis is constructed based on selected conference papers and articles, therefore note that some parts of the text might be repeated in other chapters.

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THEORETICAL FRAMEWORK

The intense competition in global market leads companies to strive for the most efficient utilization of all processes. In industrial application, improvement of the currently existing product to obtain a more efficient process becomes crucial. In optimizing the current design of an existing appliance, the use of automated design and optimization process is a crucial part of the product development [1]. The rapid product design cycle leads to the exploitation of optimization methods and the development of automatic optimization tools. Hence, it is necessary to choose the most suitable method to be applied to the present numerical model. In this chapter, different optimization methods from various aspects will be explained.

2.1 CLASSIFICATION OF OPTIMIZATION METHODS

In terms of geometry, optimization methods can be classified into three types: size, shape, and topology optimization. Chapter 2.1.1 will discuss each of these optimization method. In terms of the cost function, the optimization problem can be classified into single and multi-objective optimization. In Chapter 2.1.2, the concept of Pareto front will be introduced, as well as the equation bound for the multi-objective optimization. Lastly, in terms of algorithm, zero, first, and second order optimization will be discussed in Chapter 2.1.3.

2.1.1 *Size/Shape/Topology Optimization*

In optimizing the present heat exchanger, the alteration of the geometry is the focus of this thesis. The current gas-side heat transfer surface of the pins will be modified to obtain a new optimized surface. In altering the geometry of the heat exchanger, three types of optimization are commonly employed: size optimization, shape optimization, and topology optimization [2]. The size optimization is the simplest optimization method, because only one design parameter is optimized, e.g. diameter, length, or spacing of the pins. In this case, no modification on the shape is carried out, in the sense that the original shape is maintained, but only the size is varied. A manual parametric variation can be employed for this kind of optimization, or by using a specific algorithm to find the optimum size. The manual parametric variation is commonly practiced in industry, however it has a drawback when a large number of parameters are to be studied. Another drawback of size optimization is

the large computational effort needed to solve the flow equation every time a new geometry is simulated. Furthermore, the size optimization is limited to a certain arrangement of the pins. To answer the research question formulated in the previous chapter, this type of optimization cannot be used as it is not bound to produce a new shape.

On the other hand, shape and topology optimization can offer a wider possibility of new shapes that can achieve a better performance. In practice, an optimum arrangement of fluid channels within a particular space can be obtained using the topology optimization. However, the drawback of this type of optimization is the uncommon distribution of the three-dimensional channels that leads to final intricate channels, see for example [3-11]. This adds complexity to the manufacturing process and is deemed to be unsuitable for the current heat exchanger. Topology optimization is generally used with higher manufacturing technology, as this type of optimization sets how a material fills in a space by filtering each grid cells into one of the two types of materials: fluid or solid. On the contrary, the shape optimization can be used with a more conventional manufacturing technology, as the optimization method focuses only on producing new shapes that are based on a change of internal or external boundaries. Particularly, the type of material for each grid cells has been predetermined and only the location of the boundaries are modified.

In the present heat exchanger case, the external boundaries of the pins are the subject of the shape optimization method, while the topology or the arrangement of the pins within the boiler space is not considered to be optimized. To take into account the internal arrangement of the pins, a size optimization is first carried out in this work to find the best possible arrangement. Afterwards, the shape optimization is performed for such an arrangement. The results of the two-steps optimization is given in Chapter 6. Additionally, using this two-steps optimization method, a relatively manufacturable geometries can be produced with conventional methods (e.g. by casting) compared to the geometries obtained from the topology optimization.

2.1.2 *Single and Multi-Objective Optimization*

In terms of cost function, the optimization problem is classified into single and multi-objective optimization. In the real life application, the design of the device usually involves a consideration of multiple objectives, such as both the heat transfer between different media and the mechanical pumping power needed to move the fluid through the device [12]. The current heat exchanger case is considered as a multi-objective optimization problem with the end goal consisting of more than two objectives, e.g. heat transfer, pressure drop, material volume, and emission. However, for the current work in this thesis, a maximum

of two objectives is considered, namely the heat transfer maximization and either pressure drop or drag force minimization.

Before performing the multi-objective optimization, single objective optimization is performed for both the heat transfer and the pressure drop separately, and the effect of optimizing one of the two to the other observable is noted (the result of this study is presented in Chapter 5). In this subchapter, the concept of single and multi-objective optimization will be explained, as well as the combination of two objectives into a single cost function and the Pareto concept.

The formulation of the multi-objective optimization problem is expressed in the following:

$$\begin{aligned}
 \text{Minimize: } & f_i(\vec{x}) & i = 1 \dots l \\
 \text{Subject to: } & g_j(\vec{x}) \leq 0 & j = 1 \dots m \\
 & h_k(\vec{x}) = 0 & k = 1 \dots n \\
 & x_p^l(\vec{x}) \leq x_p \leq x_p^u(\vec{x}) & p = 1 \dots q
 \end{aligned} \tag{2.1}$$

with $f_i(\vec{x})$ being the objective function (or cost function) to minimize, and $\vec{x}$ is the vector of design variables. Since the term 'cost function' and 'objective function' are generally used interchangeably, in this thesis the differentiation of these terms will be clarified. From this point onward, the term 'objective' refers to either heat transfer, pressure drop, or drag force that is being optimized. The term 'cost function' refers to the mathematical formulation where both objectives are combined into a single equation to be minimized (or one objective equation for the single objective optimization case). Another term is introduced as 'observable', which is used only for the single objective optimization case. In the single objective optimization, only one 'objective' is being the parameter of interest, while the other non-optimized parameter will be referred to as 'observable'.

Other terms in equation 2.1 are explained as follow: the term $g_j(\vec{x}) \leq 0$ is the so-called inequality constraints, and $h_k(\vec{x}) = 0$ is the equality constraints. Note that m and k should be ≥ 0 . If m and k are equal to 0, the problem is considered as an unconstrained optimization problem.

The choice of objective function $f_i(\vec{x})$ is important in determining the resulting shape of the optimization problem. For the multi-objective optimization of the present heat exchanger, this means that the designer should choose an objective function that satisfies both the heat transfer and pressure drop requirements. Since heat transfer and pressure drop are two contradicting observables, optimizing designs that best manage trade-offs between these two conflicting criteria is a very critical issue [13]. The trade-off between two or more conflicting criteria is best visualized in the so-called *Pareto front* [14]. A set of solutions that are non-dominated construct the Pareto front, as shown in Figure 2.1.

Figure 2.1: Illustration of the Pareto front for the current multi-objective optimization. The non-dominated designs are marked by the blue dots on the Pareto front. The grey area represents dominated designs, which can be optimized. The arrow shows the direction of the improvement.

The design points located on the Pareto front are the best designs in terms of heat transfer and pressure drop. Along the Pareto front, the designer can see how much is the trade-off between the heat transfer and the pressure drop, e.g. how much the heat transfer is reduced for a design with a lower pressure drop, and vice versa. The area under the Pareto front represents the design area where the heat transfer and pressure drop are not fully optimized. The direction of the optimization is marked by the arrow pointing towards a higher heat transfer and lower pressure drop. Thus, most multi-objective optimization processes aim to construct the Pareto front so that the decision maker can choose the solution point according to one's preference.

To combine both heat transfer and pressure drop into the objective function $f_i(\vec{x})$, several ways can be employed. Some methods to combine more than one objective into a single objective function are, among others, the weighted sum method, the constrained single objective optimization, and the min-max method [15]. For the current work, the weighted sum method is chosen. The weighted sum method, based on linear combination of the objective functions, is a suitable method for identifying the Pareto front [16]. The weighted-sum approach can obtain the convex part of the Pareto front by progressively varying the weight factor values in the aggregated objective function formulation [17]. However, this method has a drawback that the ideal weights are evaluated through a time-consuming trial and error process, resulting in different optimum solutions with various degrees of constraint violation, as shown in Wu and Liu [18]. Nevertheless, this method is used throughout this thesis and the influence of the weights to the design solutions are studied.

2.1.3 *n*-th order optimization

In improving the existing appliance, several optimization methods can be employed. As previously stated, the most commonly used method in industry is the manual parametric optimization, in which the geometry of the appliance is varied by repeatedly changing its value and performing the simulation to solve the flow state in the new geometrical arrangement. Example of works on parametric optimization can be found in [19-24] for both circular and elliptical cylinders.

A more efficient way to optimize than running a parametric optimization is by using a certain algorithm to obtain the best pin arrangement. Ge et al. [25] used multi-objective optimization using the zero-order genetic algorithm to find the optimal pin arrangement by varying the spacing between the pins. Note this kind of procedure is categorized as the size optimization. Other widely-used application of optimization algorithm is to perform shape optimization for a specific array arrangement. Hilbert et al. [26] and Ranut et al. [27] performed shape optimization procedures of an array of circular and elliptical cylinders using genetic algorithm, while Cheng and Chang [28] designed shapes with inverse heat transfer method.

In performing shape optimization, three types of algorithms can be employed: gradient-free (zero-order), gradient-based (first order), and Hessian-based (second-order) algorithms [29]. The choice of algorithms depends on the complexity of the optimization method. The gradient-based methods are usually more accurate than gradient-free methods since they exploit the information of the gradient of the function [27, 30]. This method is suitable for problems with large number of design variables. The computation of the objective function gradients is independent of the number of design variables and the computational cost for solving the adjoint sensitivity is roughly the same as for solving the flow equations. In this thesis, the gradient-based adjoint method is used for the current multi-objective shape optimization. The results of this optimization procedure are generated in the form of new optimized shapes. The performance of the new shapes is then compared to that of the original geometry in terms of pressure drop and heat transfer.

Looking at the attractiveness of adjoint method, this method is deemed suitable for the current heat exchanger optimization in which the heat transfer, pressure drop, material volume, emission, and cost are to be optimized. In this thesis, only the heat transfer and pressure drop or drag force are optimized. Furthermore, the low Reynolds flows in the heat exchanger are simulated using steady simulations. Low Reynolds flows is characterized by the absence of the von Kármán vortex shedding, allowing the laminar model to be applied for the adjoint optimization. This laminar model gives limitation to the current study in a manner that the realistic application of the heat exchanger

would have the flow at around $Re_D = 500 - 2000$. In this flow regime, the strong von Kármán vortex shedding will require the unsteady adjoint simulation. However, it is computationally expensive to apply the adjoint method to the unsteady flow since the adjoint computation depends on the result of the flow simulation. Moreover, the higher number of objectives will also add more complexity to the model. Due to this limitation, the adjoint optimization is done at only two Reynolds : $Re_D = 10$ and $Re_D = 100$ in Chapter 4-6. Furthermore, only two objectives are optimized in this study, namely the pressure drop (or drag force) and the heat transfer. In Chapter 7, although the Reynolds number refers to the periodic flow, due to the staggered arrangement of the cylinder, a steady flow is obtained. Hence, the adjoint optimization can be employed for this case. The discussion on the challenges that arise for this particular case is presented in Chapter 7.

2.2 ADJOINT METHOD IN ANSYS FLUENT

In performing the adjoint shape optimization in ANSYS Fluent, the user has to follow through a procedure as depicted in Figure 2.2.

The process starts with solving the flow equations for the initial geometry. The governing equation of the mass and momentum conservation are formulated subsequently as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (2.2)$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} + \vec{F} \quad (2.3)$$

For the momentum conservation, p is the static pressure, τ is the stress tensor, and $\rho \vec{g}$ and $\vec{F}$ are the gravitational body force and external body forces (for example, that arise from interaction with the dispersed phase and other user-defined source), respectively. The stress tensor τ is related to the strain rate by:

$$\tau = \mu \left(\nabla \vec{v} + \nabla \vec{v}^T - \frac{2}{3} \nabla \cdot \vec{v} I \right) \quad (2.4)$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

The energy equation is written in the following equation:

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot (k_{eff} \nabla T + (\tau_{eff} \cdot \vec{v})) \quad (2.5)$$

Figure 2.2: Workflow of the current adjoint shape optimization procedure in ANSYS Fluent. Closed loop indicates the automatic process.

where k_{eff} is the effective conductivity ($k + k_t$), with k_t being the turbulent thermal conductivity according to the turbulent model being used (no turbulent model is used in this thesis, thus $k_t = 0$). The two terms on the right-hand side of the equation represent the energy transfer due to conduction and viscous dissipation, respectively.

The term E is defined as follows:

$$E = h - \frac{p}{\rho} + \frac{1}{2}v^2 \quad (2.6)$$

where sensible enthalpy h for incompressible flow is:

$$h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (2.7)$$

Equation 2.5 includes pressure work and kinetic energy terms, however these terms are neglected in the computation when a pressure-based solver is used [31]. In addition to that, the viscous dissipation term is neglected as viscous heating is often negligible for a flow with Brinkman number $Br \ll 1$.

For the calculation of the fluid side's heat transfer at a wall, the Fourier's law is applied. Thus, the heat flux q is computed as:

$$q = k_f \frac{\partial T}{\partial n} \quad (2.8)$$

where k_f denotes the fluid-side conductive heat transfer coefficient and n is the local coordinate normal to the wall.

After computing the flow, the sensitivities of the objectives are obtained from the adjoint calculation. The computation of the adjoint solution starts with the sensitivity derivatives of the objective J . The objective J is a function of the flow state q and the physical boundary c . The change in the location of the boundary leads to the change of the objective,

$$\delta J = \left[\frac{\partial J}{\partial q} \right] \delta q + \left[\frac{\partial J}{\partial c} \right] \delta c \quad (2.9)$$

The change of the governing flow equation $R(q, c)$ can also be expressed by the flow state q and the physical location of the boundary c ,

$$\delta R = \left[\frac{\partial R}{\partial q} \right] \delta q + \left[\frac{\partial R}{\partial c} \right] \delta c \quad (2.10)$$

When convergence is achieved, for an infinitesimal change of design variable, δR equals zero. Thus, adding this term into equation 2.9 will not change the result. Introducing a Lagrange multiplier ψ [32], equation 2.9 can be rewritten as

$$\begin{aligned}\delta J &= \left[\frac{\partial J}{\partial q} \right] \delta q + \left[\frac{\partial J}{\partial c} \right] \delta c - \psi^T \left(\left[\frac{\partial R}{\partial q} \right] \delta q + \left[\frac{\partial R}{\partial c} \right] \delta c \right) \\ \delta J &= \left(\frac{\partial J}{\partial q} - \psi^T \left[\frac{\partial R}{\partial q} \right] \right) \delta q + \left(\frac{\partial J}{\partial c} - \psi^T \left[\frac{\partial R}{\partial c} \right] \right) \delta c\end{aligned}\quad (2.11)$$

The Lagrange multiplier ψ is arbitrary and can be chosen such that the first term in equation 2.11 is eliminated. Eliminating the first term in the right-hand side of the equation 2.11 implies that the gradient of the objective function is now dependent only on design variable without needing to solve the changes of flow state for each design variable repeatedly. In order to do so, the Lagrange multiplier ψ is chosen such that it satisfies the adjoint equation

$$\left[\frac{\partial R}{\partial q} \right]^T \psi = \left[\frac{\partial J}{\partial q} \right]^T \quad (2.12)$$

Thus, the large number of design variables can be taken into account by solving the adjoint equation. This approach is attractive for large number of design variables since the additional computational time is only needed for solving the adjoint equation. Finally, equation 2.11 becomes

$$\delta J = \left(\frac{\partial J}{\partial c} - \psi^T \left[\frac{\partial R}{\partial c} \right] \right) \delta c \quad (2.13)$$

For each design iteration, the solutions of the flow equations and the adjoint equation are required. The adjoint equation is computed to determine the direction of the improvement based on the sensitivity δJ , which will be used as the basis of the mesh morphing process. The sensitivities of the objectives with respect to the shape are formulated as:

$$\delta J = \left[\frac{\partial J}{\partial c_j^n} \right] \delta c_j^n \quad (2.14)$$

with ∂c_j^n is the j^{th} coordinate of the n^{th} node of the mesh. For the morphed mesh, an arbitrary factor λ is added for the $(i+1)^{th}$ design iteration:

$$\delta c_j^n = \lambda \left[\frac{\partial J}{\partial c_j^n} \right] \quad (2.15)$$

such that a new mesh coordinate is obtained for the optimized geometry. Here λ is the objective step size specified by the user and can be chosen as a positive or negative value depending on the minimization or maximization of the objective. The choice of the objective step size is crucial. Too small a step size leads to poor convergence rate of the optimization procedure, while too large a step size may cause the optimization procedure to overshoot the nearest optimum [30]. The objective step sizes λ also serve as weight factors for the multi-objective optimization case, by making it dimensionless with respect to the initial objective $J_i(c)$. Afterwards, the optimizer will compute the change of the objectives according to the specified step sizes before morphing the mesh.

This iterative procedure for the mesh morphing is basically the application of the so-called steepest descent method to approach the optimal solution:

$$c_{i+1} = c_i - \lambda \frac{\partial J}{\partial c} \quad (2.16)$$

with i being the design iteration. The step size can be obtained by a line search procedure [33], in which the user needs to do a trial and error to test whether the chosen step size results in a reduction of the cost function. In the current work, fixed step sizes are chosen for the entire optimization procedure for an automated process in ANSYS Fluent. The step sizes are chosen to be sufficiently small such that the optimization process can approach the optimum point as close as possible. Using a fixed step size can provide reasonable solutions for unconstrained problems [16], however it is unknown whether using these chosen, fixed step sizes are good enough to approach the optimum point of the current optimization case. The study of an adjustable step size is not within the scope of this thesis since it requires a manual setting within the loop of Figure 2.2 and is left for future work.

After the step size is chosen, the mesh is morphed accordingly. The mesh morphing process occurs only for selected mesh elements that are located within a *bounding box*. The bounding box is a region where all the mesh points within this region are morphed. Within the bounding box, a number of *control points* are located equidistantly. Two sets of control points are created to map the movement of the control point to the grid points: one according to Bernstein polynomial, and one according to B-spline [31]. The Bernstein polynomial is used to control the large-scale deformation, while the B-spline is used for the fine-scale motion. The formulation of the Bernstein polynomial of degree l is presented as follow:

$$B_{i,l}(u) = \begin{bmatrix} l \\ i \end{bmatrix} u^i (1-u)^{(n-i)} \quad (2.17)$$

The i^{th} B-spline of degree p is the non-periodic B-spline that uses a knot-vector, $\{t_i\}$, where:

$$t_i = \begin{cases} 0 & i \leq p \\ \frac{(i-p)}{(l-2p)} & p < i < l-p \\ 1 & i \geq l-p \end{cases} \quad (2.18)$$

The value of B-spline is defined as:

$$S_{i,0}(t) = \begin{cases} 1 & t_i < t < t_{i+1}; t_i < t_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (2.19)$$

$$S_{i,j}(t) = \frac{t - t_i}{t_{i+j} - t_i} S_{i,j-1}(t) + \frac{t_{i+j+1} - t}{t_{i+j+1} - t_{i+1}} S_{i+1,j+1}(t)$$

Finally, the displacement of the mesh points are carried out by the superposition of the displacement of the control points associated with the Bernstein polynomial and the displacement of the control points associated with the B-spline. All the mesh points within the bounding box are subjected to this morphing scheme. The new shape is obtained after the boundary mesh points are deformed according to the aforementioned procedure.

After modifying the shape, the primal flow solver should be re-run and the new, improved objective is acquired. From this point on, this procedure will be referred to as one *design iteration*, starting from the attainment of the primal flow solution to the next convergence of the primal flow solution of the improved geometry. If the objectives are improved, the process is repeated for the next design iteration. If the objective is not improved, usually due to the too large of a step size, the optimization cycle is stopped. Aside from the too large step size, the process can also be stopped if the mesh quality falls below a certain value (typically lower than 0.1), or if the mesh morphing process results in negative cells due to the overlapping of the adjacent mesh elements. When this happens, the last geometry obtained is taken as the final optimized geometry and is remeshed to improve the mesh quality. Finally, the flow is recomputed for the remeshed geometry to confirm the improvement of both objectives, and the shapes obtained from this remeshed geometry is determined as the final optimized shape.

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Part II

3D SINGLE CYLINDER

In the second part of the thesis, results involving three-dimensional model of a single cylinder are presented.

DIRECT NUMERICAL SIMULATION OF FLOW AND HEAT TRANSFER OVER A CIRCULAR CYLINDER

In this chapter, the results of the direct numerical simulation of flow and heat transfer over a circular cylinder at $Re_D = 2000$ will be presented. This flow regime represents the high Reynolds flow at the bottom of the Bosch heat exchanger. Note that no adjoint shape optimization is performed for this model.

ABSTRACT Unsteady direct numerical simulations of the flow around a circular cylinder have been performed at $Re_D = 2000$. Both two-dimensional and three-dimensional simulations are validated with laminar cold flow simulations and experiments. Heat transfer simulations are carried out and the time-averaged local Nusselt number at the cylinder surface is obtained for various Reynolds numbers. Finally, the heat transfer of 2D and 3D simulations are compared. The average Nusselt numbers are found to be in accordance with empirical correlations. The 3D simulation gives a higher heat transfer due to the captured effects of motions in the spanwise direction compared to the 2D simulation. The irregular fluctuation of surface-averaged Nusselt number can be captured by the 3D simulation, while 2D simulation results show a regular fluctuation corresponding to the shedding from the cylinder, similar to that of a laminar flow.

3.1 INTRODUCTION

Transitional flow around a cylinder has been studied extensively due to its flow characteristics. Shear layer instability, different patterns of vortex streets, and shedding frequency are among the flow characteristics that are subject to investigations. Research by means of numerical as well as experimental work has been done in the past to understand the flow behavior that is neither fully laminar nor fully turbulent. The current work is focused on the direct numerical simulation of the flow and heat transfer at $Re_D = 2000$. The flow at $Re_D = 2000$ portray the transition regime perfectly, as it undergoes a transformation from a lower transition in shear layer to an intermediate transition in shear layer [1]. As the name suggests, this regime is marked by the instability

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at the shear layer, a region close to the cylinder where the boundary layers continue to develop downstream.

To the authors' knowledge, the closest study to $Re_D = 2000$ was done by Norberg [2] who conducted a smoke visualization to capture the bi-stable flow. It was noted that the vortex street switches from the regular Strouhal mode to the irregular mode due to the condition of the end plate. Aside from that, a 2D DNS of cold flow at $Re_D = 2000$ has been performed by Braza et al. [3]. Other works in the regime close to $Re_D = 2000$ can be found in Wei and Smith [4], who observed experimentally the development of the spanwise shear layer at $Re_D = 2400$. Prasad and Williamson [5] conducted a study at $Re_D = 2500$ which results in a correlation between the shear layer frequency and the von Kármán frequency. Kravchenko and Moin [6] have performed large eddy simulations at $Re_D = 3900$. Wissink and Rodi [7] used the results of this work together with experimental results of Lourenco and Shih [8] at the same Reynolds number as a basic test case for their direct numerical simulations. They carried out simulations at $Re_D = 3300$, which are the closest direct numerical simulation to the current work as of the authors' knowledge. They studied the near wake of a circular cylinder at $Re_D = 3300$ by numerical means, resulting in a detailed phase-averaged statistics of the rolled up shear layers that are originated from the boundary layers. Other numerical simulations at lower Reynolds number have been performed by Mittal [9] using a time-dependent, three-dimensional model. His simulations at $Re_D = 1000$ suggest that the 2D results tend to overestimate the Strouhal number and mean drag coefficient than the 3D simulation. Aside from numerical simulations, considerable experimental studies at Reynolds number around 2000 have been realized using hot wire anemometry and flow visualization. The readers are referred to the works of Gerrard [10] at $Re_D = 2000$ and Kourta et al. [11] for $Re_D = 2660, 2150$. At $Re_D = 3900$, several experiments has been performed [12, 13], as well as numerical simulations [6, 14, 15].

The flow at $Re_D = 2000$ is considered to lie in the low Reynolds regime for the transitional flow, hence most of the engineering applications at this Reynolds number employ two-dimensional simulations to reduce the computational cost. The 2D simulation is beneficial for the fully laminar flow, as the flow is dominated by two-dimensional motions, thus a two-dimensional simulation is sufficient to capture the flow physics accurately. However, as the three dimensional motions start to affect the flow with increasing Reynolds number, it is deemed important that a three-dimensional simulation is used for Re 250 and higher [6]. One characterization of the transitional flow at this regime is the existence of the secondary vortices in the shear layer. The primary von Kármán vortices are shed at a certain frequency which corresponds to the Strouhal number $\frac{St=fD}{u}$. As the Reynolds number increases, the

boundary layer develops and the onset of turbulence is observed to be originated from the separated shear layer. According to Bloor and Gerard [16], these 'transition waves' are manifested as Tollmien-Schlichting waves along the separated shear layer and are responsible for enhancing the heat transfer. To the authors' knowledge, no detailed 3D heat transfer simulation has been performed at this low Reynolds of the transition regime. One of the main aims of this work is to study the differences between 2D and 3D DNS at relatively low Reynolds number in terms of heat transfer and flow. In this chapter, the effects of three-dimensional motions to the flow and heat transfer at $Re_D = 2000$ will be explained in terms of the development of Nusselt number at the cylinder surface over time.

3.2 METHODOLOGY

In this section, the governing equation and the numerical setup for the DNS cases will be explained.

3.2.1 Governing Equations

The instantaneous equation of mass and momentum conservation are formulated subsequently as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (3.1)$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} + \vec{F} \quad (3.2)$$

For the momentum conservation, p is the static pressure, τ is the stress tensor, and $\rho \vec{g}$ and $\vec{F}$ are the gravitational body force and external body forces (for example, that arise from interaction with the dispersed phase and other user-defined source), respectively. The stress tensor τ is related to the strain rate by:

$$\tau = \mu \left(\nabla \vec{v} + \nabla \vec{v}^T - \frac{2}{3} \nabla \cdot \vec{v} I \right) \quad (3.3)$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

The energy equation is written in the following equation:

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot \left(k_{eff} \nabla T + \left(\tau_{eff} \cdot \vec{v} \right) \right) \quad (3.4)$$

where k_{eff} is the effective conductivity ($k + k_t$), with k_t being the turbulent thermal conductivity according to the turbulent model being used. The two terms on the right-hand side of the equation represent the energy transfer due to conduction and viscous dissipation, respectively.

The term E is defined as follows:

$$E = h - \frac{p}{\rho} + \frac{1}{2}v^2 \quad (3.5)$$

where sensible enthalpy h for incompressible flow is:

$$h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (3.6)$$

Equation 3.4 includes pressure work and kinetic energy terms, however these terms are neglected in the computation when a pressure-based solver is used [17]. In addition to that, the viscous dissipation term is neglected as viscous heating is often negligible for a flow with Brinkman number $Br \ll 1$.

For the calculation of the fluid side's heat transfer at a wall, the Fourier's law is applied. Thus, the heat flux q is computed as:

$$q = k_f \frac{\partial T}{\partial n} \quad (3.7)$$

where k_f denotes the fluid-side conductive heat transfer coefficient and n is the local coordinate normal to the wall.

For a fixed temperature boundary condition applied at the wall, the heat transfer coefficient and subsequently, surface Nusselt number are calculated as follows:

$$h = \frac{q}{(T_{wall} - T_{in})} \quad (3.8)$$

$$Nu = \frac{hD}{k_f} \quad (3.9)$$

The Nusselt number is averaged over the cylinder surface for one period of von Kármán vortex shedding. This period is referred to as the 'Strouhal period' from this point onward. The time-averaged Nusselt numbers obtained from the 2D and 3D DNS are then compared to empirical correlations for flow around a cylinder. The readers are referred to Churchill and Bernstein [18], Hilpert [19], and Zukauskas

Table 3.1: List of constants for time-averaged Nusselt number correlations.

Re_D	C [19]	m [19]	C [20]	m [20]
0.4 – 1	0.989	0.330	0.75	0.4
1 – 4	0.989	0.330	0.75	0.4
4 – 40	0.911	0.385	0.75	0.4
40 – 1000	0.683	0.466	0.51	0.5
1000 – 4000	0.683	0.466	0.26	0.6

[20]. Churchill and Bernstein proposed a correlation for all Re_D for $Pr \geq 0.2$, with all properties are evaluated at film temperature, $(T_{in} + T_{cyl})/2$.

$$Nu_D = 0.3 + \frac{0.62(Re_D)^{\frac{1}{2}} Pr^{\frac{1}{3}}}{\left[1 + \left(\frac{0.4}{Pr}\right)^{\frac{2}{5}}\right]^{\frac{1}{4}}} \left[1 + \left(\frac{Re_D}{282000}\right)^{\frac{5}{8}}\right]^{\frac{4}{5}} \quad (3.10)$$

The correlation of Hilpert [19] is formulated in Equation 3.11 for $Pr \geq 0.7$ with all properties evaluated at film temperature.

$$Nu_D = C Re_D^m Pr^{\frac{1}{3}} \quad (3.11)$$

Correlation by Zukauskas [20] is shown in Equation 3.12 with all properties evaluated at T_{in} and Pr_s at the cylinder surface.

$$Nu_D = C Re_D^m Pr^n \left(\frac{Pr}{Pr_s}\right)^{\frac{1}{4}} \quad (3.12)$$

The constants C and m of Hilpert and Zukauskas are listed in Table 3.1.

3.2.2 Numerical Setup

3.2.2.1 2D DNS

The two-dimensional numerical domain is depicted in Figure 3.1. Two regions are created: Region I that is close to the cylinder with a fine mesh and Region II with a coarser mesh. The cylinder with diameter D is located $10D$ from the inlet and $30D$ from the outlet. A no slip boundary condition and temperature of 289.16 K is employed at the cylinder wall. Uniform velocity U_0 with temperature of 288.16 K is imposed at the inlet. It is assumed that the effects of temperature on

Figure 3.1: Computational domain for the 2D simulation.

the fluid properties are negligible, thus constant fluid properties are used. At the top and bottom boundaries of the domain, slip boundaries are used.

The two-dimensional simulation is performed using 1.4 million quadrilateral elements. At the cylinder wall, 1600 elements are placed equidistantly with 500 inflation layers growing in the radial direction (Figure 3.2). The height of the inflation layer is chosen such that there are 5 layers inside the boundary layer. The front-stagnation-point boundary-layer displacement thickness is calculated according to Schlichting [21],

$$\delta_{FSP} = \frac{0.67}{2(Re_D)^{\frac{1}{2}}} D \quad (3.13)$$

Based on the mesh study that have been carried out, the maximum size of the elements in Region I is specified to be $0.1D$, while the maximum size of elements in Region II is $0.2D$. The size of the smallest elements on the wall of the cylinder is $0.0005D$.

3.2.2.2 3D DNS

The size of the three-dimensional domain is the same as the two-dimensional domain, with $10D$ length in the spanwise direction (Figure 3.3). This length is chosen based on the results of Wissink and Rodi [7] who suggested that the spanwise length should be longer than $8D$ to fully capture the motions in the spanwise direction. The three-dimensional domain consists of two regions with different mesh elements. Region I consists of triangular mesh with hexahedral inflation elements surrounding the cylinder. Region II consists of hexahedral elements with face size of $0.002D$ and $0.004D$ length in the spanwise direction. Note that the inflation elements close to the cylinder surface

Figure 3.2: (a) Inflation layer close to the cylinder. Note that only the tenth grid lines are shown here due to the dense grid. (b) Transition from the inflation layers to the quadrilateral elements.

is very fine and the hexahedral elements are fine enough to bridge the inflation region and Region II. Using this setting, the total number of elements is 13.9 million.

The structured and finer elements employed in this region are necessary to capture the fluctuation of the three-dimensional flow at multiple points in the wake region, as well as the Kolmogorov length scale η ,

$$\eta = \left(\frac{\nu^3}{\bar{\xi}} \right)^{\frac{1}{4}} \quad (3.14)$$

Finally, the Kolmogorov length scale for this simulation is calculated to be in the order of $0.003D$.

3.2.2.3 Numerical schemes

The numerical simulations have been performed using ANSYS Fluent 16.0. The governing equations are discretized using the semi-implicit finite volume method. The gradients are evaluated using the least squares cell-based method, and the second order upwind scheme is employed for the spatial discretization of the pressure term, while the third order discretization is used for momentum equation and energy equation [17]. The transient term is discretized using a second order scheme. The time step applied in this simulation is $8 \times 10^{-4}D/u$.

Figure 3.3: (a) Computational domain for 3D simulations. (b) Transition from the inflation layers to the triangular and hexahedral elements.

3.3 RESULTS

3.3.1 Validation

To validate the numerical model, a cold laminar flow is simulated. The Strouhal number is obtained as a function of Reynolds number and the results are plotted in Figure 3.4. The results of 2D simulations are in the same order of the experimental results of Hammache and Gharib [22] and Williamson [23]. At Reynolds higher than approximately 170, the 2D simulation continues showing the increasing trend of the curve. At this Reynolds number, the flow becomes three dimensional and thus the sudden drop of the Strouhal number cannot be matched by the 2D simulation. The 3D simulation result is also in a good agreement with

Figure 3.4: Results of validation for laminar cold flow. The 2D simulation is well within the experimental values and the 3D simulation result matches the results of Hammache and Gharib [22].

literature, e.g. at $Re_D = 100$, the Strouhal number is found to be within 5% difference compared to both experimental values.

3.3.2 Results of heat transfer simulations for 2D laminar flow

The heat transfer simulation is performed with the 2D domain for low Reynolds numbers: 10, 45, and 100. The local Nusselt number is averaged over one period of vortex shedding and is plotted along the surface of the cylinder (Figure 3.5). The results of 2D simulation are found to be in accordance with numerical simulations of Bharti et al. [24] at $Re_D = 10$ and $Re_D = 45$.

The mean Nusselt number increases with increasing Re_D and the local Nusselt number $Nu(\theta)$ is maximum at the front stagnation point. This corresponds well with the trend of increasing Nu with higher Re from literature. A local minimum value indicates the separation point. The location of the separation point moves towards the front of the cylinder with increasing Reynolds number [24]. Simulations at $Re_D = 45$ and $Re_D = 100$ are in a good agreement with this trend, showing the separation point at $\theta = 137.9^\circ$ and $\theta = 136.4^\circ$ subsequently.

3.3.3 Comparison of 2D and 3D simulation at $Re = 2000$

The mesh resolution of the 2D domain is sufficient to capture the secondary vortices, as shown in Figure 3.6. Two separation points are visible; these cause the formation of secondary vortices at the free shear layer. This flow pattern is in accordance with the description of the flow

Figure 3.5: Time-averaged local Nusselt number at the cylinder surface as a function of θ for 2D simulation. $\theta = 0^\circ$ corresponds to the front stagnation point.

at $Re_D = 2000$ by Braza et al. [3]. The 3D domain also shows a sufficient mesh resolution as shown in Figure 3.7. The axial velocity is plotted for ten axial locations in the longitudinal center plane. The normalized results are compared with that of Wissink and Rodi [7] at $Re_D = 3300$. As investigated by Wissink and Rodi, an insufficient mesh will result in a V-shaped profile close to the cylinder. Although both simulations are conducted at different Re_D , the velocity profiles are similar. The U-shaped profile for the line closest to the cylinder indicates that the current numerical simulation has enough mesh resolution.

The 2D simulation cannot capture the effects of spanwise motion, as shown in Figure 3.8. The instantaneous vorticity fields at $t = 1049U_0/D$ are compared. The 2D simulation results in a regular flow pattern instead of uneven eddies. Moreover, the widening of the wake region is immediately visible in the near wake from the 3D simulation. Accordingly, the surface-averaged Nusselt number at the cylinder wall is plotted as a function of flow time and the results correspond well with the flow field. As the turbulence flow is captured by the 3D simulation, the surface-averaged Nusselt number fluctuates irregularly. On the contrary, the 2D simulation shows a regular oscillation of surface-averaged Nusselt number due to the regular shedding of the vortices. The time-averaged surface Nusselt numbers from both simulations are computed and the results are plotted in Figure 3.9. The 3D simulation gives a higher heat transfer compared to 2D flow due to the higher turbulence of the flow and this is within 5% difference compared to the empirical correlation of Zukauskas [20].

The development of local Nusselt number along the cylinder surface is shown in Figure 3.10. From Figure 3.10a at $t = 0.25T$ and approxi-

Figure 3.6: Instantaneous vorticity field of the 2D simulation. Separation points and secondary structures (red arrows) are visible.

Figure 3.7: Profile of u -velocity in 10 lines, taken at the center plane of the cylinder. Solid lines represent current simulations; dashed lines represent results of Wissink and Rodi at $Re = 3300$ [7].

mately $\theta = 240^\circ$, a local maximum indicates that the heat transfer at the back of the cylinder is enhanced by the lower recirculating vortex while its pair is shed from the upper part of the cylinder. Half a period later, the local maximum at $\theta = 120^\circ$ indicates that the recirculating vortex now appears at the upper part of the cylinder while the lower vortex is shed. On the contrary, the 3D simulation does not show a regular pattern of local Nusselt number due to the influence of the spanwise motions. Figure 3.10b shows the local Nusselt number taken at plane $Z = 0$. After one period, the local Nusselt profile at $\theta = 90^\circ$ to $\theta = 270^\circ$ does not repeat the same pattern. From the front stagnation point ($\theta = 0^\circ$) to $\theta = 90^\circ$ and $\theta = 270^\circ$, there are no significant differences between 2D and 3D simulations. However, at $\theta = 90^\circ$ to $\theta = 270^\circ$

Figure 3.8: Instantaneous flow field and surface-averaged Nusselt number for (a) 2D simulation and (b) 3D simulation at $t = 1049U_0/D$.

Figure 3.9: Time-averaged, surface-averaged Nusselt number of current results compared to empirical correlations [18-20].

the 3D turbulent eddies at the back of the cylinder causes the change of local Nusselt number with time. Thus, the 3D simulation results in a higher time-averaged Nusselt number.

The instantaneous vorticity fields from the 3D simulations are shown in Figure 3.11. In the first frame the vortex at the bottom of the cylinder is being shed. The subsequent frame depicts the formation of the upper vortex while the lower vortex shrinks. In the next image, the upper vortex is being shed and finally shrinks in the following frame. The movement in the spanwise direction is also visible as an undulation of the curling eddies attached to the cylinder wall. The shedding of the von Kármán vortex street is still visible in each frame, marked by eddy filaments rolling in a form of sheets parallel to the cylinder axis.

Figure 3.10: Time-averaged local Nusselt number as a function of θ for (a) 2D simulation and (b) 3D simulation. $\theta = 0^\circ$ corresponds to the front stagnation point.

Figure 3.11: Instantaneous isocontour of swirling strength of $37.9/s$, taken at $865.6D/U_0$, $867.6D/U_0$, $869.6D/U_0$ and $871.6D/U_0$.

3.4 SUMMARY

2D and 3D simulation have been performed for laminar and transitional flow. Both cold flow and hot flow simulations are found to be in accordance with literature. Compared to 2D simulation, the time-averaged Nusselt number in the 3D simulation is higher due to the turbulence development and this value is within 5% difference of empirical correlations. Thus, a two-dimensional domain can be used to simulate heat transfer case at $Re_D = 2000$ when engineering accuracy is sufficient.

However, at $Re_D = 2000$ the flow is irregular due to the shedding in the spanwise direction. These movements can be captured well by the 3D simulation and results in a fluctuation of surface-averaged Nusselt number over time. Thus, to perform a detailed statistical flow analysis, a 3D simulation is of a paramount importance.

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3D MULTI-OBJECTIVE OPTIMIZATION OF SINGLE CYLINDER WITH CONJUGATE HEAT TRANSFER

There are uncertainties whether ANSYS Fluent's adjoint can handle transitional flow at $Re_D = 2000$. ANSYS Fluent's adjoint has some modeling limitations particular for this operating condition of Bosch heat exchanger. First of all, unsteady adjoint is currently not available in ANSYS Fluent. Furthermore, for turbulent flow modeling, a frozen turbulence assumption is used [1]. This means that the effect of changes to the state of the turbulence is not taken into account when computing the sensitivities, hence the optimized shape is obtained only for a particular state of flow. Another concern should be considered regarding ANSYS Fluent adjoint's limitation for the conjugate heat transfer case. In this case, the solid body is supported but it should be noted that this body should not use a moving reference frame approach [1]. Furthermore, problems such as stiff convergence and non-accurate prediction of the observables are also known to happen for cases using the following turbulence model: $k - \varepsilon$, $k - \omega$, and $k - \omega - SST$ model [2]. Considering these limitations and potential problems, it is therefore concluded that the model in Chapter 3 is too complex for starting the ANSYS Fluent adjoint optimization. As the results in Chapter 3 suggest, the flow at $Re_D = 2000$ has developed turbulence in the shear layer. Moreover, three-dimensional effects have started to appear at this Reynolds number. To conduct the first shape optimization study of the adjoint procedure, the Reynolds number is lowered up to $Re_D = 10$ to maintain the laminar flow and to avoid instabilities due to vortex shedding.

ABSTRACT A cylinder in a cross-flow is modeled and optimized using the discrete adjoint method in ANSYS Fluent 18.2. The circular cylinder is bounded at both ends and a constant temperature boundary condition is imposed at one end. The conduction in the solid body of the cylinder as well as the convective heat transfer to the laminar flow are solved. The heat transfer and the drag force at the cylinder surface are optimized and the shapes resulting from the optimization procedures are compared with the initial geometry. Due to the conductive heat transfer along the length of the cylinder, different shapes are obtained along the cross-section of the cylinder. The results show that the area close to the front and rear stagnation points do not undergo a significant

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change, while the area around the 45° and 135° angle of the cylinder are gradually deformed. Furthermore, the area close to the root of the cylinder is not deformed significantly, while the largest deformation occurs in the middle length of the cylinder. Finally, the optimized cylinder can achieve 1.9% increase of heat transfer and -2.4% decrease of drag force.

4.1 INTRODUCTION

Circular cylinder is commonly used for industrial application. One example of such application is for heat transfer enhancement in a heat exchanger. Hence, the flow and heat transfer around a circular cylinder in a cross-flow has been a widely studied subject. Various efforts have been carried out to find optimum arrangements of circular cylinder array within a confined space to optimize the heat transfer. An overview of parameters effect on the heat exchanger performances can be found in Kays and London [3] for compact heat exchangers. Lee et al. [4] obtained the optimal shape and arrangement of staggered cylinders in a channel using a parametric study, while Ge et al. [5] carried out a multi-objective optimization using genetic algorithm to find the optimum arrangement of a cylinder array. Adjoint method has only been recently used for heat transfer optimization, e.g. in the work of Wang et al. [6] who performed size optimization for a fin of a heat exchanger using the discrete method.

All these works employ a parametric study to find the optimal arrangement, while maintaining the shape of the pin/fin and increasing the performance of the thermofluid system. To the authors' knowledge, no study about shape optimization of a circular cylinder with conjugate heat transfer using the discrete adjoint optimization has been performed in the past. The closest study is that of Ranut et al. [7], who performed a two-dimensional zero-order genetic algorithm for shape optimization of a circular cylinder. In this thesis, the adjoint approach is used rather than the genetic algorithm due to its better accuracy since it exploits the information of the gradient of the function directly [7, 8]. The adjoint method is used for the shape optimization of a single cylinder in a cross-flow to optimize the heat transfer and the drag force. Furthermore, the three-dimensional effect of conduction along the length of the cylinder is taken into account using the conjugate heat transfer model. Due to this effect, different shapes result from the optimization procedure.

4.2 METHODOLOGY

In this chapter, the interaction between solid and fluid domain in terms of heat transfer will be modeled. The term *conjugate heat transfer* will be used from this point onward to refer to this kind of process which

involves variation of temperature within the two bodies due to thermal interaction between them [9]. Thus, the energy equation at the interface of the solid and fluid bodies [10] is formulated as:

$$\nabla \cdot (k \nabla T)_{fluid} = \nabla \cdot (k \nabla T)_{solid} \quad (4.1)$$

The gradient-based adjoint method has been developed since the work of Jameson [11] and Pironneau [12]. Here the discrete adjoint method is used, where the discrete adjoint equations are derived from the discretized form of the flow equation. The computation of the adjoint solution starts with the sensitivity derivatives of the objective J . The objective J is a function of the flow state q and the physical boundary c . The change in the location of the boundary leads to the change of the objective,

$$\delta J = \left[\frac{\partial J}{\partial q} \right] \delta q + \left[\frac{\partial J}{\partial c} \right] \delta c \quad (4.2)$$

The change of the governing flow equation $R(q, c)$ can also be expressed by the flow state q and the physical location of the boundary c ,

$$\delta R = \left[\frac{\partial R}{\partial q} \right] \delta q + \left[\frac{\partial R}{\partial c} \right] \delta c \quad (4.3)$$

When convergence is achieved, for an infinitesimal change of design variable, δR equals zero. Thus, adding this term into equation 4.2 will not change the result. Introducing a Lagrange multiplier ψ [12], equation 4.2 can be rewritten as

$$\begin{aligned} \delta J &= \left[\frac{\partial J}{\partial q} \right] \delta q + \left[\frac{\partial J}{\partial c} \right] \delta c - \psi^T \left(\left[\frac{\partial R}{\partial q} \right] \delta q + \left[\frac{\partial R}{\partial c} \right] \delta c \right) \\ \delta J &= \left(\left[\frac{\partial J}{\partial q} \right] - \psi^T \left[\frac{\partial R}{\partial q} \right] \right) \delta q + \left(\left[\frac{\partial J}{\partial c} \right] - \psi^T \left[\frac{\partial R}{\partial c} \right] \right) \delta c \end{aligned} \quad (4.4)$$

The Lagrange multiplier ψ is arbitrary and can be chosen such that the first term in equation 4.4 is eliminated. Eliminating the first term in equation 4.4 implies that the gradient of the objective function is now dependent only on design variable without needing to solve the changes of flow state for each design variable repeatedly. In order to do so, the Lagrange multiplier ψ is chosen such that it satisfies the adjoint equation

$$\left[\frac{\partial R}{\partial q} \right]^T \psi = \left[\frac{\partial J}{\partial q} \right]^T \quad (4.5)$$

Thus, the large number of design variables can be taken into account by solving the adjoint equation. This approach is attractive for large number of design variables since the additional computational time is only needed for solving the adjoint equation. Finally, equation 4.4 becomes

$$\delta J = \left(\frac{\partial I}{\partial c} - \psi^T \left[\frac{\partial R}{\partial c} \right] \right) \delta c \quad (4.6)$$

For each design iteration, the solutions of the flow equations and the adjoint equation are required. The adjoint equation is computed to determine the direction of the improvement and the mesh is morphed accordingly while taking into account the input step size for the objectives [1]. For the details of the mesh morphing procedure, readers are referred to Chapter 2. The cycle is repeated to obtain a new optimized shape with each design iteration.

For the current optimization, both the heat transfer and the drag force are optimized. The weighted sum method [13] is used to construct the objective function for this multi-objective optimization:

$$U = \sum_{i=1}^n w_i J_i(c) \quad (4.7)$$

where weight factor $w_i > 0$ and U is the multi-objective function to minimize. For a comprehensive review on the choice of the weights and methods to optimize the weights, the readers are referred to [14, 15, 16].

4.3 NUMERICAL SETUP

The computational domain used in this study is shown in Figure 4.1. A single cylinder with diameter D is placed in a crossflow with one end embedded in an aluminum plate. At the bottom of the plate, constant temperature and convective heat transfer boundary conditions are imposed. The top of the domain is set as a no slip, adiabatic wall, while the side planes are set as a symmetry boundary condition. At the inlet, a flow with $Re_D = 10$ and $1K$ temperature higher than the base plate are imposed. The choice of $Re_D = 10$ was used to avoid unsteady flow due to vortex shedding. The length of the cylinder is chosen in accordance with the domain in Chapter 3. The outlet is set as a pressure outlet boundary condition.

The three-dimensional model consists of 2.7 million elements. At the cylinder wall, 400 elements are placed equidistantly with 50 inflation layers growing in the radial direction with growth ratio of 1.033 and first layer thickness of $0.0002m$. 50 elements are set along the span of

Figure 4.1: Computational domain and boundary conditions.

the cylinder with increasing element density near both ends, while 8 elements are placed along the thickness of the solid base plate.

The numerical simulation is performed using ANSYS Fluent 18.2. For the primal solver, the governing equations are discretized using the pressure-based coupled algorithm [10]. The gradients are evaluated using the Green-Gauss Cell Based method and the second order upwind scheme is employed for the spatial discretization of the pressure term, momentum, and energy equation. The standard discretization scheme is used for the pressure term of the adjoint equation and the first order upwind scheme for the adjoint momentum and energy equation. A laminar flow model is used for solving the low Reynolds number of the flow.

4.4 RESULTS

4.4.1 Sensitivity Vectors

The results of the flow solution and adjoint solution are shown in Figure 4.2. The temperature contour shows higher temperature at the tip of the cylinder, while the root temperature is close to the imposed temperature boundary condition, 288.16K. Accordingly, from the viewpoint of the cylinder span, the magnitude of the shape sensitivity vector for heat transfer increases towards the tip of the cylinder. Figure 4.2b shows the wall effect near the root and the tip of the cylinder that affects the magnitude of the sensitivity vectors at these locations. If one consider only the temperature contour in Figure 4.2a, the highest deformation should occur at the tip of the cylinder. However, due to the wall friction near the tip of the cylinder, the shape sensitivity magnitude is lower at the tip, but not as low as the root of the cylinder. Consequently, the highest sensitivity magnitude occur at the middle length of the cylinder.

Figure 4.2: (a) Temperature profile along the length of the cylinder. (b) Vector of shape sensitivity magnitude for heat transfer at the surface of the initial geometry, visualized for the spanwise length of the cylinder. The wall effect can be seen at the tip (left end) and the root (right end) of the cylinder. (c) Vector of shape sensitivity magnitude for heat transfer, skipped every 10 cells for better visualization.

Figure 4.3: Vector of sensitivity magnitude for body force (drag) at the surface of the initial geometry, with the top view shown to depict the inward direction of the deformation.

The direction of the deformation corresponding to the heat transfer optimization is shown by the arrows pointing outwards of the cylinder body (Figure 4.2c). The highest deformation occurs around the front stagnation point of the cylinder, as indicated by the red arrows. Next to this area of highest deformation, the sensitivity vector appear to be minimum as depicted by lack of arrows and the dark blue arrows at the upper and lower part of the cylinder. This means that this area will not undergo a significant deformation to improve the heat transfer. The back of the cylinder have a relatively uniform magnitude of the vector, indicating that the deformation will occur outward, but less than that of the front stagnation point.

The shape sensitivity vector for the drag force shows that highest drag occurs at around the front stagnation point, as indicated by the red arrows (Figure 4.3). Contrary to the heat transfer adjoint vectors, some sensitivity vectors show inwards direction at the front part of the cylinder, indicating that the deformation should occur towards the solid body. Furthermore, the sensitivity vectors corresponding to the drag force optimization are symmetric with respect to the middle length of the cylinder due to the wall boundary conditions at both ends. This is represented by absence of the high-magnitude vectors near both walls.

Considering the magnitude of the sensitivity vectors for both observables along the length of the cylinder, one could predict that the highest deformation will occur at the middle length of the cylinder. This hypothesis is proven in the next subsection.

Figure 4.4: *Top*: Top view of the optimized cylinder. The overlaying cross sections are marked by the black lines. *Middle*: The upper front deformation of the cylinder at 45° angle. *Bottom*: The upper rear deformation of the cylinder at 135° angle.

4.4.2 Final Optimized Shape

The shapes resulting from the adjoint optimization are depicted in Figure 4.4, where the three-dimensional deformation of the cylinder is shown. The top view of the cylinder shows overlaying cross sections, marked by the black regions. The area close to the front and rear stagnation points do not undergo a significant change, while the area around the 45° and 135° angle of the cylinder are gradually deformed, shown by the 'pinched' surface in Figure 4.4. Note that $\theta = 0^\circ$ refers to the front stagnation point. At $\theta = 45^\circ$, the solid surface is deformed both outwards (into the fluid domain) and inwards (into the solid domain), while at $\theta = 135^\circ$, the deformation is mainly outwards. No constraint is imposed on the surface area or on the movement of the mesh points.

Figure 4.5 shows the different cross sections of the optimized cylinder. Since the drag force is relatively constant along the length (with the exception near the root and the tip of the cylinder due to the wall boundary condition where the drag force is highest), the effect of conduction along the length of the cylinder can be seen. The area close to the root and the tip of the cylinder is not deformed significantly, while the largest deformation occurs in the middle of the cylinder span.

Using this optimized geometry, one can achieve 1.9% increase of heat transfer and -2.4% decrease of drag force. The development of the

Figure 4.5: Results of the optimization procedure: different cross sectional shapes along the length of the cylinder. $Z = 0$ represents the root of the cylinder, while $Z = 0.1$ represents the tip of the cylinder. The cross sections of the root and the tip are exactly the same as the initial geometry. Flow is from the left.

Table 4.1: Evaluation of the expected, realized, and calculated value of heat transfer and drag force for the optimized geometry. The expected value is obtained from the sensitivity calculation of the adjoint solver, realized value from the recalculation of the flow after mesh deformation (CFD solver), and calculated value is from the summation of (realized+expected) value.

Iter.	Heat transfer (W)				Drag force (N)			
	Exp'd	Real. (E-02)	Calc. (E-07)	Off (%)	Exp'd	Real. (E-07)	Calc. (E-07)	Off (%)
0		-1.249				8.8663		
1	-1E-05	-1.251	-1.2504	-0.011	-1E-10	8.7096	8.8653	1.787
2	-5E-05	-1.256	-1.2555	-0.054	-1E-10	8.7090	8.7086	-0.004
3	-5E-05	-1.262	-1.2612	-0.038	-1E-10	8.7090	8.7080	-0.009
4	-5E-05	-1.266	-1.2667	0.026	-1E-10	8.7083	8.7078	-0.006
5	-5E-05	-1.273	-1.2714	-0.121	-1E-08	8.6517	8.5827	-0.797

objectives with respect to the design iteration is presented in Figure 4.6 and Table 4.1.

The results of the adjoint optimization shows that an optimized shape can be obtained although the prediction of the objectives is not 100% accurate, resulting in discrepancy between the calculation from the adjoint solver and the calculation from the flow (CFD) solver as presented in Table 4.1. In this table, the expected value refers to the expected change obtained from the adjoint calculations. The realized values are the one obtained from the CFD recomputation after the mesh is deformed (see flowchart in Figure 2.2). The calculated value is obtained from the summation of the expected value and the realized value of the previous design iteration. The percent of error is defined as the dif-

Figure 4.6: Development of heat transfer and drag force over the design iteration.

ference between the calculated and the realized value. Table 4.1 shows that the error margin is within 0.12% for the heat transfer. However, larger error is observed for the drag force up to 1.8%. Nevertheless, with this relatively large error, a decent solution can still be achieved by the adjoint optimization procedure which improves both heat transfer and drag force.

The results of this three-dimensional optimization serves as a starting point before performing the three-dimensional optimization for an array of cylinders in cross-flow. This case will be discussed further in Chapter 7.

4.5 SUMMARY

Using adjoint optimization procedure in ANSYS Fluent, a three-dimensional conjugate heat transfer model of a cylinder in a cross-flow is optimized. The optimized geometry shows the effect of conduction in a solid body by the different shapes emerging for different cross sections along the length of the cylinder. The final optimized geometry can achieve 1.9% increase of heat transfer and -2.4% decrease of drag force.

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Part III

2D ARRAYS

In the third part of the thesis, results involving two-dimensional models of arrays of circular and non-circular cylinders are presented.

2D SINGLE AND MULTI-OBJECTIVE OPTIMIZATION OF CYLINDER ARRAYS

The results presented in the preceding chapter show that the ANSYS Fluent adjoint optimization procedure is able to produce a new optimized shape for a 3D geometry. However, some difficulties were encountered when determining the weight factors for both objectives. As mentioned in literature, the ideal weights are evaluated through a time-consuming trial and error process. This makes the total time needed for the optimization process to become longer. To reduce the time needed for the trial and error process, a study on the influence of heat transfer or pressure drop optimization to the non-optimized observable is carried out with a two-dimensional domain. Two single objective optimizations are performed to know its effect on the non-optimized observable. Using the result of these optimizations, the user can select approximately the suitable weight factors for the multi-objective optimization.

ABSTRACT A 2D model of a pin-fin heat exchanger is optimized using the discrete adjoint method in ANSYS Fluent 16.0. The initial heat exchanger shape is modeled as staggered cylinders in a cross-flow. Two observables are monitored during the optimization cycles: the heat transfer and the pressure drop, and the objectives are the maximization of heat transfer and the minimization of pressure drop. However, improving the performance of the heat exchanger poses its own challenges since the heat transfer and pressure drop are usually two contradicting observables. In order to successfully improve both observables, single objective and multi-objective shape optimizations are studied. Both single and multi-objective optimizations are conducted under steady laminar flow conditions at $Re_D = 10$ and $Re_D = 100$. For single objective optimizations, one observable is optimized while the change of the unconstrained observable is monitored. The single objective optimizations are done for different step sizes of the geometry change, e.g. different changes of pressure drop or heat transfer. The optimized observable behaves linearly, while the other unconstrained observable shows a nonlinear deterioration. The multi-objective optimizations are performed for different weight factors, leading to different end shapes. For the final optimized geometry, up to 11% reduction in pressure drop and 11% increase in heat transfer is achieved.

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5.1 INTRODUCTION

Optimization of heat transfer and pressure drop in a heat exchanger has been a subject of extensive study. This subject poses its own challenges since the heat transfer and pressure drop are usually two contradicting observables. Moreover, the large number of design variables contributes to the large amount of computational time needed to perform the parameter study. Considering these restrictions, gradient-based methods are often used to compute the gradient of the objective function with respect to the design variables. To compute the gradient of the objective function, the adjoint approach is more efficient compared to other methods, such as direct sensitivity analysis [1]. The adjoint method has a low computational cost since it does not depend on the number of the design variables. Consequently, the computational cost is roughly the same as for solving the flow equations [2].

Some examples of the utilization of the adjoint method in optimization cases can be found in [3], who performed a size optimization of a fin of a heat exchanger. The fin height, length, pitch, and width are optimized to minimize the drag force. Other studies involving multi-objective optimization and conflicting observables using the adjoint method have been carried out in the field of topology optimization [4, 5, 6, 7, 8]. Oevelen and Baelmans [4] reduced the thermal resistance of a heat sink while maintaining a certain pressure drop. Kontoleon et al. [5] used the adjoint method to minimize pressure drop and maximize the temperature rise inside a duct. Other duct optimization was carried out by Villiers and Othmer [6] to optimize pressure drop and flow swirl. Marck et al. [7] minimized the pressure drop and maximized the recoverable thermal power of a channel/pipe, while Haertel et al. [8] maximized the heat transfer of a heat sink while maintaining a certain pressure drop.

To the author's knowledge, no studies about shape optimization of cylinder arrays using the adjoint method for heat transfer and pressure drop are reported in the literature. In this chapter, we discuss the shape optimization of cylinder arrays with respect to heat transfer and pressure drop. The heat transfer and pressure drop evolution with every shape change resulting from adjoint optimization will be evaluated. Finally, the optimized shape for the cylinder array will be presented and compared.

5.2 METHODOLOGY

The single objective optimization is done under steady laminar flow conditions for both $Re_D = 10$ and $Re_D = 100$. Two Reynolds numbers are chosen to see the effect of the design change when the flow state is changed. Each observable is optimized separately, while the other

non-constrained observable is monitored and its development over the design iteration is noted. Firstly, a study to determine the optimum step size is carried out to ensure the behavior of the optimized observable. A too large step size will result in a large mesh deformation, leading to inconsistent behavior prone to poor prediction of the optimized observables. Since the step size is kept constant over the design iteration, the optimized observable should improve linearly. The single objective study is important to ensure this behavior, as well as to monitor the unconstrained observable and to obtain its relation with the optimized observable. Moreover, the chosen step size also serves as weight factors for the multi-objective optimization. The step size study through the single objective optimization could give an indication about the weighting of each observable during the multi-objective optimization.

The relation between the step size, number of design change, and the optimized observable for the single objective optimization should fulfill the following equation:

$$y = \frac{s}{I_0}n + 1 \quad (5.1)$$

with $y = I_n/I_0$. Note that n is the number of design iteration, I_0 is the initial heat transfer or pressure drop, and s refers to the step size. This equation holds for the optimized observable, while the relation between the other unconstrained observable to the number of design iteration is sought. These correlations will be compared for the two flow conditions.

From the single objective optimization, one could determine the weight factors for the multi-objective optimization. The weighted sum method [9] is used to construct the objective function for the multi-objective optimization:

$$U = \sum_{i=1}^n w_i J_i(c) \quad (5.2)$$

where weight factor $w_i > 0$ and U is the multi-objective function to minimize.

5.3 COMPUTATIONAL DOMAIN

The computational domain and boundary conditions are shown in Figure 5.1. The geometry consists of a staggered array of pins with $D = 10mm$. The longitudinal and transversal pitches are subsequently $S_T/D = 2$ and $S_L/D = 1$. Using the meshing tool from ANSYS [10], the number of inflation layers, number of division at the cylinder surface, relevance, and relevance center are varied. The inflation layers are used

Figure 5.1: Computational domain and boundary conditions. Dimensions in *mm*.

Table 5.1: List of different meshes. Quality 1 and skewness 0 indicate the best mesh.

Mesh	Settings				Statistics			
	Inflation layer	Divi- sion	Relevance center	Rele- vance	No. of elements	Ortho. quality	Ortho. skew	Aspect ratio
A	2	20	Fine	100	1343	0.53	0.41	4.77
B	5	100	Fine	100	5181	0.52	0.42	5.66
C	10	200	Fine	100	16993	0.68	0.27	3.71
D	20	400	Fine	100	57269	0.38	0.20	7.57
E	20	400	Max. el.	1.25mm	123617	0.24	0.44	7.58

to capture the boundary layer in the vicinity of the cylinder, while the number of circular divisions determines the degree of complexity of the cylinder surface that can be obtained by the adjoint optimization. The relevance and relevance center influence the global size of the elements and the degree of mesh refinement. Relevance is defined as the most basic global size control and its value is set between -100 and 100, with a negative value coarser than a positive value [10]. The relevance center sets the mid point of the relevance slider control, with three options: coarse, medium, and fine. Relevance 100 and relevance center 'fine' refers to the finest mesh. Another way to perform mesh refinement is by controlling the mesh element size, in which one has to specify the maximum size of the element. Different meshes are studied and its specifications are listed in Table 5.1.

The mesh study is done at $Re_D = 100$. The inlet temperature is set at 288.16K and 1K higher at the cylinder surface. Constant fluid properties are used. A second order upwind scheme is used for both momentum and energy discretization.

Figure 5.2 shows several properties obtained at different locations within the domain. The pressure and temperature profiles are taken at line $x = 0D$ and $x = 4D$. The effect of the mesh at the vicinity of the cylinder is shown by the local wall shear stress and the heat transfer

Figure 5.2: Result of mesh study: (a) pressure profile and (b) temperature profile of the fluid at different locations. (c) Wall shear stress and (d) local heat transfer coefficient, taken at the surface of the left-most cylinder.

coefficient at the cylinder surface. The coarse meshes (mesh A and B) result in a significant difference compared to the finer meshes (mesh C, D, E). For the mesh morphing purpose, 400 circular divisions at the cylinder surface are chosen. As there is no significant difference between mesh C, D, and E, finally mesh D is chosen due to its small number of elements and its lowest skewness.

5.4 RESULTS

5.4.1 Single Objective Optimization

The results of the single objective optimization process for heat transfer is shown in Figure 5.3. The convergence plot is shown in terms of the ratio of the modified to the initial value of the observables. As heat transfer is optimized, it is shown that after around 100 design iterations, there is no significant change of heat transfer or pressure drop with increasing number of iteration. Thus, this simulation is referred to as 'converged' in terms of shape change. The end shape of the optimized geometry is shown in Figure 5.3b, compared to the initial

geometry (Figure 5.3c). The temperature contour plot indicates that the temperature of the fluid domain increases with the new optimized shape.

Figure 5.4 shows the final optimized shape of the pressure drop optimization. As opposed to heat transfer optimization, the final shapes deform such that the fluid channel is enlarged, resulting in a lower velocity magnitude than the initial geometry. Furthermore, a tear-drop shape is observed, especially at the front and the rear end of the middle cylinder due to the attempt of the adjoint procedure to morph the mesh towards a flat plate shape, and finally towards an empty channel. The left-most and right-most cylinders have a rounded section around the front and the rear stagnation point due to the constraint of the bounding box which limits the movement of the mesh points.

Figure 5.5 shows the development of both observables over the design iterations. Note that the optimized geometry in Figure 5.3b refers to Figure 5.5a and Figure 5.4a refers to Figure 5.5b. Figure 5.5 shows that the optimized observable behaves linearly, while the other unconstrained observable shows a nonlinear deterioration with respect to the number of design iteration. For the optimized observable, the same gradient

Figure 5.3: (a) Typical convergence plot of single objective optimization for heat transfer at $Re = 100$ and temperature contour of the final optimized shape of heat transfer optimization taken for HT $-1e - 02$ at iteration 101 (b) compared to the initial geometry (c).

Figure 5.4: Velocity contour plot of: (a) Final optimized shape of pressure drop optimization compared to (b) initial geometry.

is obtained with different step sizes, suggesting that these step sizes are sufficiently small to reproduce the linear behavior of the observable. However, there are some discrepancies, e.g. in Figure 5.5a, due to the deterioration of the mesh quality at the 35th iteration. The deterioration is caused by the large number of design cycles while there is no mesh refinement performed during the optimization process.

5.4.2 Multi-Objective Optimization

The multi objective optimizations are performed according to the step sizes found in Section 5.4.1. For the heat transfer, a step size of $1e-02W$ and $1e-03W$ are sufficient to obtain repeatable behavior, while the step sizes for pressure drop are $1e-02Pa$ and $1e-03Pa$. Comparing Figure 5.3a and Figure 5.5b, one could conclude that the heat transfer optimization can be run roughly 7 times longer than the pressure drop optimization (200 iterations vs 30 iterations for the same step size $1e-02$). This information suggests roughly 1 order of magnitude difference between the heat transfer and pressure drop weight factors to achieve a multi-objective optimization where the relative improvements are comparable. Moreover, the improvement of heat transfer is relatively small compared to that of the pressure drop, indicating that the heat transfer should be given more weight to achieve a successful optimization of both observables. To check this, several runs with different weight factors are carried out and the results are shown in Figure 5.6.

Figure 5.6 depicts the development of the observables within an objective space. The aim is to obtain improvement for both objectives which could be used to construct the Pareto front. The starting point of the initial design is marked by the coordinate (1,1) and the different lines result from different weight factors.

Most of the simulations are able to achieve improvement for both heat transfer and pressure drop, except case 2 and 4. Case 2 uses the same step size for both objectives and from the results it can be seen

Figure 5.5: Results of single objective optimization: (a) heat transfer optimization and (b) pressure drop optimization for $Re_D = 100$. (c) Heat transfer optimization for $Re_D = 10$, heat transfer shows 0.1% improvement. (d) Pressure drop optimization for $Re_D = 10$. Step sizes in $[W, Pa]$. The linear correlations of the optimized observables are in accordance with Equation 5.1. Furthermore, the unconstrained observables show different trends for different flow conditions, as shown by the nonlinear curve fitting equations in Figure 5.3. Unlike the $Re_D = 100$ cases, non-quadratic curve fittings are imposed to the $Re_D = 10$ cases to obtain the most suitable correlation for the unconstrained observable behaviors.

that the weight is put more to the pressure drop, hence suggesting that the step size for pressure drop is too large. When more weight is given to the heat transfer (case 4), the heat transfer is optimized up to 11% at the expense of 2% increase in pressure drop. Two cases are run using the same weight factors but different step sizes: case 1 and 3. Both lines are intersecting, leading to the same end point of the optimized geometry. The effect of different weight factors can be seen more clearly in Figure 5.6b. The angle between the heat transfer and pressure drop lines represents the different weight factors.

The relative step sizes for case 3 are scaled to $Re_D = 10$, resulting in case 5. As a comparison, an even larger step size in pressure drop gives more optimization on the pressure drop, while the change in heat transfer is negligible (case 6). For $Re_D = 10$, a different mesh is used

Figure 5.6: (a) Trajectories of multi-objective optimization in the objective space. The simulations start at initial design (1,1) and develop over the lines. Markers placed at every 10 design iterations. (b) The development of both objectives per design iteration for different weight factors. Heat transfer step sizes are in W , while pressure drop in Pa .

Figure 5.7: Final optimized shapes for $Re_D = 100$. Starting from the top-left figure, clockwise: case 2 compared to initial geometry, case 3 compared to initial geometry, comparison of case 1 and 3 that have the same weight factors, and case 4 compared to case 3.

which is finer and has a better quality. The inlet length is also closer to the cylinders to reduce the computational time. The change of inlet length does not give a significant effect on the converged flow state.

Figure 5.7 show the final, optimized geometry for the two flow conditions. For the cases of $Re_D = 100$, the geometries show a similar trend for all pins. Case 2 gives the narrowest pins to reduce the pressure drop, particularly the sharp front edge of the middle and rear cylinders. The end shape of case 2, 3, and 4 are similar. Cases with the same weight factors lead to the similar end shape (Figure 5.7c). Case 4 leads to shorter edges of the half-cylinders and more rounded full-cylinders to obtain high heat transfer (Figure 5.7d). In terms of flow velocity, the optimized shapes lead to a more uniform flow (Figure 5.8).

Figure 5.8: Velocity contour plot of the initial geometry (a) compared to the optimized geometry of case 3 (b). Note that the maximum velocity is reduced, leading to a more uniform bulk flow.

Figure 5.9: Final optimized shape for $Re_D = 10$, case 5 (a) and case 6 (b). The mesh is deformed such that the left-most cylinder moves towards the inlet. At the border of the bounding box, the mesh points are cluttered, causing sharp edges for the left-most cylinder.

In comparison, the results of $Re_D = 10$ optimization give a larger shape change for the front pin. As can be seen in Figure 5.9, the effect of bounding box can be seen as it limits the movement of the mesh points. Due to the bounding box, there are points at the symmetry boundary of the geometry which are constrained and cannot move during the mesh morphing process, hence the sharp indentation at the top and at the bottom of the half-cylinders for $Re_D = 100$ and the sharp edges at the left-most cylinder of $Re_D = 10$ (Figure 5.10). The sharp edges and the cluttering of the mesh points may deteriorate the mesh quality, leading to premature termination of the automatic optimization process. This problem will be addressed in the next chapter to obtain the most optimum geometry without constraining the edge of the boundaries.

5.5 SUMMARY

Single and multi-objective optimizations have been done at $Re_D = 10$ and $Re_D = 100$ for an array of cylinders using the adjoint method in ANSYS Fluent. The geometry step size for each observable is studied using the single objective optimization. Optimum step sizes are found for each observable that ensure the consistency of the improvement. Us-

Figure 5.10: Example of the bounding box placement relative to the cluttered mesh points for (a) case 5 at $Re_D = 10$ and (b) case 4 at $Re_D = 100$.

ing these step sizes, the multi-objective optimization can be successfully carried out.

From the single objective optimization, the applied step size is sufficiently small such that the optimized observable behaves linearly, while the other observable behaves non-linearly with respect to the number of design iterations. The multi-objective optimization algorithm in Fluent works such that both objectives are optimized in a linear behavior, suggesting that there is enough room for improvement in the design space. The relation between heat transfer and pressure drop is found for each single objective optimization. Different step sizes result in the same correlation, while different flow conditions result in different correlations.

The multi-objective optimization results in a different progress of improvement with different weight factors. Different end shapes are obtained for $Re_D = 10$ and $Re_D = 100$. As a comparison, for the runs that use the same weight factors, the final optimized geometry of $Re_D = 100$ gives 11% reduction in pressure drop and 11% increase in heat transfer, while the final optimized geometry of $Re_D = 10$ results in 11% reduction in pressure drop and 4% increase in heat transfer. These cases need to be further studied as the simulations are automatically stopped due to the significant reduction in mesh quality caused by the fixed mesh points.

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2D PARAMETRIC AND SHAPE OPTIMIZATION OF CYLINDER ARRAYS AND ADJOINT PARAMETER ANALYSIS

In this chapter, the two-dimensional adjoint optimization of the cylinder arrays are discussed in more detail. Both parametric size optimization and adjoint shape optimization are performed. Furthermore, influence of adjoint parameters such as initial geometry, domain size, bounding box, and control points to the end geometry are analyzed and presented.

ABSTRACT A 2D model of a pin-fin heat exchanger is studied numerically for an automatic optimization procedure. The initial heat exchanger shape is modeled as staggered cylinders in a cross-flow. Increasing the performance of such a device possesses its own challenges since heat transfer and pressure drop are two contradicting objectives. Therefore, a new optimization strategy for heat transfer and pressure drop is proposed for the optimization of an array of cylinders in a cross-flow. First, a conventional parameter study of the array is performed to construct the Pareto front. Subsequently, two geometries close to the Pareto front are chosen as starting geometries for the gradient-based optimization procedure in ANSYS Fluent 18.2. Using the discrete adjoint method, the multi-objective optimization is done for both circular cylinder and ellipse array to find a new optimized shape. For each of the arrays, the effects of different weight factors with respect to the performance and to the end geometry are studied. The results show that the geometries resulting from the adjoint optimization procedure can achieve better performance beyond the conventional Pareto front. Finally, a remeshing procedure of the final optimized geometries is done to validate the computed heat transfer and pressure drop.

The effect of optimization paths in the objective space to the geometries is studied. Several geometries resulting from intersecting paths are compared. Furthermore, the effects of the domain sizes are also studied to eliminate the indentation problem that exists in the previous chapter. It is found that the imposed symmetry boundary conditions could be the cause of the indentations. This problem could not be eliminated unless by enlarging the bounding box. Hence, the effects of the bounding box enlargement as well as the effect of the number of control points within the bounding box are studied. Finally, the different optimization cases that are represented by different domain sizes, different bounding

box sizes, different number of control points, and different symmetry boundary conditions are presented in this chapter.

6.1 INTRODUCTION

Pin-fin heat exchangers are frequently used in a broad range of applications in industry. One example of the pin-fin heat exchanger application is in the gas boiler industry. In order to reduce the production cost and increase the performance of such appliance, various efforts have been carried out in the field of heat exchanger optimization. Heat transfer enhancement, reduction of pressure drop, emission, and material volume are some examples of the optimization goals. To achieve these goals, modification of the existing appliance is commonly carried out. Adding physical structure such as winglets and fins can manipulate the flow by introducing vortex-induced flow or enhancing the heat transfer. Other mean of increasing the heat transfer is by adding heat-enhanced particles to the flow field. In this chapter, no physical structure is added, nor the fluid is changed. This chapter focuses on the design alteration of the geometry of the current heat exchanger.

In altering the geometry of the heat exchanger, three types of optimization are commonly employed: size optimization, shape optimization, and topology optimization [1]. Of the three, size optimization is the most straight forward, as one optimizes one particular parameter only, e.g. diameter, length, or spacing of the pins. As has been demonstrated in the work of Wang et al. [2], the optimum size for a fin is obtained using a specific algorithm. This method provides a good insight into all the possibilities for a certain arrangement. However, for a large number of parameters, performing this task takes a large computational effort. Moreover, size optimization is limited in the sense that the layout of a heat exchanger arrangement has to be predetermined.

On the other hand, topology optimization offers a wider possibility of arrangement by optimizing how geometries can fill in a space. In practice, an optimum arrangement of a fluid channel can be obtained using this type of optimization. However, the drawback of this method is the uncommon distribution of three-dimensional channels that leads to final intricate channels, see for example [1, 3-9]. This adds complexity to the manufacturing process and is deemed to be unsuitable for the current heat exchanger. Therefore, the current heat exchanger optimization procedure is performed using the shape optimization.

The choice of using shape optimization method is made due to the fact that the shape optimization compromises the other two types of optimization methods. Unlike the size optimization and topology optimization, shape optimization can work for geometries with a predetermined arrangement of pins. The shape optimization focuses only on each of the pin shapes, therefore increasing the performance by

keeping an orderly arrangement of the pins. This leads to relatively manufacturable geometries that can be produced with conventional methods, e.g. by casting.

In performing shape optimization, three types of algorithms can be employed: gradient-free, gradient-based, and Hessian-based algorithms [10]. The choice of algorithms depends on the complexity of the optimization method. The gradient-based methods are usually more accurate than gradient-free methods since they exploit the information of the gradient of the function [11, 12]. This method is suitable for problems with large number of design variables. The computation of the objective function gradients is independent of the number of design variables and the computational cost for solving the adjoint sensitivity is roughly the same as for solving the flow equations [10, 13, 14, 15]. This work is carried out using the gradient-based adjoint method for the multi-objective shape optimization. The results of this optimization procedure are generated in the form of new optimized shapes. The performance of the new shapes is then compared to that of the original geometry in terms of pressure drop and heat transfer.

Considering that extensive work has been done in the field of pin arrangement optimization, herewith some of the works of the past are listed. The physics of flow across a bundle of pins is discussed extensively in Zdravkovich [16]. For fluid flow and heat transfer around an array of cylinders, various works in the past have been done, as early as that of Aiba et al. [17] and Hiwada et al. [18]. For array optimization, a common practice is to carry out a conventional parameter study to find the optimal arrangement. Matos et al. [19], for example, optimized the arrangement of finned circular and elliptic tubes, while Lee et al. [20] obtained the optimal shape and arrangement of staggered pins in a channel. Deepakkumar and Jayavel [21] carried out performance evaluation of mixed ellipse and circular cylinder in an array, while Visser and de Kock [22] performed fin optimization by minimizing weight (or size) with respect to heat transfer. All of these works are in the field of parametric optimization and it is highly dependent on the operating conditions and array configuration for each case, e.g. L/D , Reynolds number, temperature difference, pin diameter and pitch. Parametric optimization leads to the necessity to define a set of solutions that fit the definition of an optimum according to the decision maker. This concept is called Pareto optimality [23]. A set of solutions that are non-dominated construct the *Pareto front* [24]. Most multi-objective optimization problems are solved based on Pareto optimization with the aim of finding the non-dominated solution to construct the Pareto front. After the Pareto front is found, it is up to the decision maker to choose the solution point according to personal preference [24].

A more efficient way to optimize than running a parametric optimization is by using a certain algorithm to obtain the best pin arrangement.

Ge et al. [25] used multi-objective optimization using the zero-order genetic algorithm to find the optimal pin arrangement. Other widely-used application of genetic algorithm is to perform shape optimization for a specific array arrangement. Hilbert et al. [26] and Ranut et al. [11] performed a shape optimization procedure of an array of circular and elliptical cylinders using genetic algorithm, while Cheng and Chang [27] designed shapes with inverse heat transfer method.

Other examples of work with heat transfer and pressure drop as an objective can be seen in [3, 4, 5, 6, 28], all in the field of topology optimization in which one of the objectives is limited as a constraint and the other one is optimized. Study on objective weights and its effect to multi-objective shape optimization is carried out by Murthy et al. [29] and Baumbach [30]. None of these works employ the same geometry as the one used in this thesis.

This chapter is the continuation of the preliminary study concerning multi-objective optimization of pressure drop and heat transfer that has been done in Chapter 5. To the authors' knowledge, no studies about shape optimization of cylinder arrays using the discrete adjoint method for heat transfer and pressure drop are reported in literature. The closest studies along this line of research of shape optimization are that of He et al. [31], in which they optimized the heat transfer and pressure drop of a U-bend using OpenFOAM's adjoint optimizer, and that of Hilbert et al. [26] and Ranut et al. [11] using genetic algorithm, as well as Cheng and Chang [27] who performed inverse heat transfer method. In the current study, the circular and ellipse cylinder array geometries are used for the discrete multi-objective adjoint optimization. A new optimization strategy is proposed, in which the optimum arrangement is found first based on the constructed Pareto front. The, the selected shape is further optimized using the adjoint procedure. Using this strategy, the array of pins can be optimized beyond the parametric-Pareto front. The capability of the discrete adjoint optimization in ANSYS Fluent 18 is explored to perform shape optimization of the initial geometries (circular and elliptical cylinder array). The resulting shapes have a better performance beyond the conventional Pareto front and these shapes will be discussed in terms of the 'path' undergone by a specific geometry during optimization cycles. Subsequently, the final optimized geometry is remeshed and the total heat transfer and pressure drop is recalculated for validation. Furthermore, the effects of weight factors, domain size, bounding box size, and the number of control points on the resulting final optimized shapes are studied in this chapter. The domain size comprises the number of cylinders in the x - and y -direction. This parameter, together with the size of bounding box and the number of control points, are important parameters for the adjoint optimization procedure in ANSYS Fluent. No study about

the effect of these parameters are reported in literature. Finally, the indentation problem encountered in the previous chapter is solved.

6.2 NUMERICAL SETUP AND METHODOLOGY

Five computational domains are used in this study (Figure 6.1). The first domain $D1$ consists of seven half-cylinders in a cross-flow. The Domain $D2$ consists of seven half-ellipses to study the effect of different initial geometries to the optimization process. For the parameter study, the diameter, transversal and longitudinal pitches of the two domains are varied to construct the Pareto front. Note that the dimensions shown in Figure 6.1 correspond to the dimension of the initial cylinder and ellipse geometry that are used for the adjoint optimization procedure. The diameter of the half-ellipse is chosen such that it has a similar surface area to the half-cylinders. For the adjoint optimization procedure, the weight factors are varied for Domain $D1$ and $D2$.

The third domain is the same geometry as the one used in Chapter 5. Using this domain, different crossed-paths on the objective space are studied. The Domain $D4$ consists of six rows of cylinders in the direction of the flow to study the effect of different domain sizes in the x -direction and the effect of bounding box. Finally, the Domain $D5$ consists of multiple rows of cylinders in the y -direction to obtain the effect of different domain sizes in the y -direction and the symmetry boundary condition. The five domains are depicted in Figure 6.1 with dimension normalized to the cylinder diameter $D = 0.01m$.

The mesh study is done according to the previous one in Chapter 5. Using the same setting for the elements at the vicinity of the cylinders (inflation layers, number of elements, relevance and relevance center), the mesh for the five domains is constructed using unstructured grid. This choice is deemed more practical for the mesh adaptation during the optimization process [11]. Moreover, the freeform deformation algorithm of the current mesher in ANSYS can handle any arbitrary cell mesh type [32]. No mesh adaptation is employed during the current optimization process, although it remains for future work. The penalty of disabling the mesh adaptation can be seen after a considerably large amount of number of design iterations, where the mesh quality decreases substantially. Thus, the final geometry is remeshed after a large number of iteration steps and the recomputed flow state on this grid is compared to the final result of the final design step. The results are presented in Chapter 6.4.2.

For the primal flow solver, the governing equations are discretized using the semi-implicit finite volume method [32]. The gradients are evaluated using the Green-Gauss cell-based method, and the second order upwind scheme is employed for the spatial discretization of the momentum equation and energy equation. A standard discretization

Figure 6.1: Computational domain D1, D2, D3, D4, and D5 from top to bottom, consecutively.

scheme is used for the pressure term of both flow solver and adjoint solver. First order upwind scheme is used for both the discretization of the adjoint momentum and adjoint energy equation. A steady laminar model is used with the justification that the differences between the steady state and the transient simulations at $Re_D = 100$ are negligible (10^{-6} magnitude difference for outlet temperature, heat flux at the cylinder surface, and pressure drop). This justification is in accordance with Ranut et al. [11] who conducted their study at a higher Reynolds, 162, which results in the maximum percentage deviation on the interested values lower than 0.5%. Moreover, early studies of cylinders in tandem as the numerical study of Li et al. [33] and experimental observation of Zdravkovich [34] stated that vortex shedding always occurred behind the downstream cylinder, but not for the upstream cylinder unless the spacing between the two cylinders exceeded $3D$. In the current case,

Table 6.1: List of all bounding box sizes (m) and the control point distribution

Domain	Bounding box type	x -min	x -max	y -min	y -max	CP($x \times y$)
$D1 - 1$	slightly larger	-0.01	0.07	-0.0102	0.0002	20x5
$D1 - 2$	18x larger	-0.01	0.07	-0.01	0.08	20x20
$D1 - 3$	18x larger	-0.01	0.07	-0.1	0.08	20x60
$D1 - 4$	18x larger	-0.01	0.07	-0.1	0.08	20x90
$D1 - 5$	3x larger	-0.01	0.07	-0.02	0.01	20x15
$D2$	slightly larger	-0.01194	0.0869	-0.0127	0.0002	20x5
$D3$ [Ch.5]	tight fit	-0.006	0.05	-0.01	0.01	20x10
$D4 - 1$	18x larger	-0.006	0.066	-0.11	0.07	20x20
$D4 - 2$	3x larger	-0.006	0.066	-0.02	0.01	20x20
$D5$	slightly larger	-0.01	0.07	-0.0502	0.0102	20x30

the spacing is less than $3D$, hence it is within the range of a steady state solution.

The gradient-based adjoint method used here is based on the work of Jameson [35] and Pironneau [36], as explained in Chapter 2. The new shape is obtained based on the mesh morphing process [32], with the bounding box size, the number of control points, and the step sizes defined by the user. The choice of weights are done by trial and error, and the readers are referred to Chapter 2 and [37, 38, 39] for further reading on the weight factors selection. A more detailed explanation about the effect of weight factors is presented in Chapter 6.4.1, where the relevance of the weights to the final optimized geometry is shown.

Different sizes of bounding boxes are used for each domain. The specifications are listed in Table 6.1. Four types of boxes are used: tight fit, slightly larger, three times and 18 times larger. The tight fit bounding box intersects with the domain at the upper and lower symmetry boundaries, thus the grid points at these boundaries cannot move. The second type of the bounding box uses a slightly larger box such that all the grid points at the upper and lower boundary of the domain are located within the box, hence the grid points are allowed to move. The 3 and 18 times larger boxes are enlarged in the y -direction. A more comprehensive explanation can be found in Chapter 6.4.5. An example of the picture of the bounding box and the domain is shown in Figure 6.2.

6.3 RESULTS

The subsequent subchapters are organized as follows: the first subchapter will discuss the effect of initial geometries. The Domains $D1 - 1$ and $D2$ are used to obtain the results in this subchapter. Different weights are employed for each of these domains. Chapter 6.4.2 describes the

Figure 6.2: Example of a slightly larger bounding box on the half-ellipse domain. Note that the clearance at the upper and lower boundaries is 0.2 mm, therefore it is not visible in this figure.

results of remeshing the final optimized geometries obtained in 6.4.1. In Chapter 6.4.3, results are presented for Domain $D3$. Chapter 6.4.4.1 and 6.4.4.2 show the results for the Domain $D1 - 2$, $D1 - 3$, $D3$, $D4 - 1$, $D4 - 2$, and $D5$ as comparison cases for the various domain sizes. Finally, the effect of the bounding box and control points are studied using the Domain $D1 - 1$, $D1 - 2$, $D1 - 3$, $D1 - 4$, and $D1 - 5$, and the results are shown in Chapter 6.4.5.

6.3.1 Effect of initial geometry and weight

To investigate the effect of weights as well as initial geometry, a parameter study is performed first. Using the Domain $D1$ and $D2$, multiple simulations are run with various cylinder diameters, ellipse axes, transversal and longitudinal pitches. The ellipse axes are varied by keeping its hydraulic diameter similar to that of the existing cylinder geometry, 10 mm. The inlet velocity is varied accordingly to keep the Reynolds number constant at 100 based on the cylinder diameter for Domain $D1$ and the hydraulic diameter for Domain $D2$. The transversal and the longitudinal pitch are varied by keeping the ratio S_T/D and S_L/D between 1.25 and 3 as it is commonly practiced for designing tube bank arrangement for heat exchangers [40, 41].

A total of 369 simulations are run while maintaining the circular and ellipse shape. The results are depicted as data points in the objective space in Figure 6.3. Afterwards, the Pareto front is constructed based on these data points. Two arrangements near the parameteric-Pareto front are selected as the initial geometry (circular and elliptical cylinder array) to be used for adjoint shape optimization. One point close to the front is chosen as a starting point for the cylinder optimization procedure (1,1). Note that this point refers to the geometry of Domain $D1 - 1$. Next, the initial half-ellipse geometry is chosen such that its performance is close to the Pareto front as well (0.32,0.77, Domain $D2$). From both points, nine shape optimization cases (A-I in Figure 6.4) are run with the adjoint optimization procedure for various weights. Hence, the different path undergone by each optimization case due to different weights can be observed.

Figure 6.3: Result of Domain $D1 - 1$ and $D2$ adjoint shape optimization in the objective space. Data points represent the parameter variation of the cylinder and ellipse geometries. Lines represent the path undergone by an initial geometry throughout the adjoint shape optimization procedure.

The weights for heat transfer and pressure drop are defined subsequently as:

$$W_Q = \frac{Q_n}{Q_0} \quad (6.1)$$

$$W_P = \frac{dP_n}{dP_0} \quad (6.2)$$

where the subscript 0 refers to the heat transfer and pressure drop of the initial half-cylinder geometry $D1 - 1$ and n is attributed to the design iteration. For every design iteration, the step sizes of pressure drop dP_n and heat transfer Q_n are kept constant in order to be able to predict the direction of the optimization in the objective space. The constant weight can give an idea about the path that will be undergone by each optimization case if a linear behavior occurs.

Due to the constant Reynolds number and varied transversal pitch, the mass flow rates and consequently the heat loads are also varying. In order to take this into consideration, a dimensionless number of thermal efficiency ratio is used. The thermal efficiency is defined as:

$$\eta = \frac{Q_{simulated}}{Q_{max}} \quad (6.3)$$

where

$$Q_{max} = mC_p dT_{max} \quad (6.4)$$

Figure 6.4: Zoomed-in result of Figure 3: Cylindrical domain D1 – 1(left) and ellipse domain D2 (right). Markers are placed every 20 design iterations. Letters A-F refer to the final optimized shape.

and the total temperature difference dT_{max} is $1K$, being the temperature difference between the inlet and the cylinders. The thermal efficiency ratio is then:

$$R = \frac{\eta_{modifiedgeometry}}{\eta_{initialhalfcylindergeometryD1}} \quad (6.5)$$

Figure 6.3 depicts the development of the observables within the objective space compared to the Pareto front obtained from the parameter study. Note that all data points are made dimensionless with respect to the initial objectives of Domain D1 – 1. Hence, the coordinate (1,1) for the initial geometry of the cylinder Domain D1 – 1 and (0.32,0.77) for the initial geometry of the half-ellipse Domain D2. In this figure, Q_n and dP_n are the step sizes in Watt and Pascal, consecutively.

The optimizations of the half-cylinders develop towards the Pareto front for some cases, and further achieve an improvement of the heat transfer beyond the front (case A, B, C). Similarly, all optimization cases of the half-ellipse develop towards better heat transfer and pressure drop (case G, H, I). The final optimized shapes consist of non-circular and non-elliptical shapes. This can be used as an optimization strategy in terms of computational time: performing a parameter variation to construct the Pareto front and subsequently performing the adjoint shape optimization only for several initial geometries located on the Pareto front. The resulting non-circular and non-elliptical shapes can achieve an improved performance beyond the conventional Pareto front. For a more detailed optimization path for each cases, Figure 6.4 shows the zoomed-in results of Figure 6.3.

Figure 6.5 shows the different final optimized geometries obtained from the Domain D1 – 1 optimization. Note that the domain is mirrored four times to give a better view on the final shape. It can be observed that the shape tend to become more round for optimization with more

Figure 6.5: Final optimized shapes for the cylinder optimization. Domains are mirrored four times to depict the shapes clearly. Note that case F represents flow at $Re_D = 10$.

weight for the pressure drop. The cylinders tend to move towards the outlet as an attempt to minimize the pressure drop by reducing the vertical distance of the upper and bottom part of the cylinders. On the contrary, due to the absence of any geometrical constraints, the freeform deformation algorithm attempts to increase the perimeter of the cylinder to enhance the heat transfer.

Figure 6.6 and Figure 6.7 show the final optimized geometries for the half ellipse optimization. The half cylinder and half ellipse case tend to give similar final shapes for weighted heat transfer or pressure drop. It was observed that for high heat transfer cases (A, B, C, G), the shapes develop towards sharp front with indentation at the rear part. This shape is similar to what is obtained in earlier study in Chapter 5 where the indentations at the top and bottom cylinders result from the constrained grid points. The constrained grid points problem is solved by enlarging the bounding box with 0.2 mm clearance to the top and bottom boundaries (see Table 6.1). The movement of the grid points at the boundary lines is set such that it can only move in the x -direction, while the rest of the grid points are allowed to move in both directions. Nevertheless, the indentation still occurs with this current setting. It could be that the shape sensitivity magnitude at the symmetry boundary lines affect the movement of these grid points. Since the sensitivities are projected into the Bernstein polynomial of degree N :

$$B_{i,N}(u) = \sum_{i=0}^N u_i \frac{N!}{(N-i)!i!} (1-u)^{(N-i)} \quad (6.6)$$

for the i^{th} grid point, hence:

$$B_{i,N}|_{x=0} = 0 \quad (6.7)$$

Figure 6.6: Differences of the shapes for final optimized geometries A, B, C (top), D, E, F (middle), and G, H, I (bottom).

Figure 6.7: Final optimized shapes for the ellipse optimization cases G, H, I.

when $i! = 0$. Note that a local (u, v) coordinate system is defined where $u \in [0, 1]$ and $v \in [0, 1]$. This local coordinate system is used for the deformation of the equally spaced array of $N_u \times N_v$ control points that is distributed within the bounding box. For the grid points at the boundary lines, there is a contribution from $B_{0,N}$ component, while the interior grid points have the contribution from all the $B_{i,N}$. The shape sensitivity at the boundaries has to be small compared to the sensitivity at the interior nodes such that it contributes to the delay of the deformation. To check this, the shape sensitivity magnitudes at the boundaries are visualized (Figure 6.8) and it is found that the magnitudes of the shape sensitivities are indeed negligible. Several high magnitude arrows pointing to opposite direction can also affect the delay of the deformation, however this is not significant due to the later smoothing for the final geometry. Finally, it is concluded that the imposed symmetry boundary condition is the main influencing factor of the delay.

For the real industrial manufacturing, one can choose the intermediate shapes to avoid the sharp edges (Figure 6.9). For example, the fifth iteration of path D results in almost the same pressure drop as the initial geometry, but with a 0.4% increase of heat transfer (see Figure 6.4 for a reference on the performance). If the manufacture process requires

Figure 6.8: Top to bottom: Shape sensitivity magnitude of: pressure drop for the cylinder surface nodes, pressure drop for the boundary nodes, heat transfer for the cylinder surface nodes, and heat transfer for the boundary nodes. Figures taken for intermediate shape at 127th design iteration of path B. Different colors of the domain boundaries represent different types of boundary conditions: blue for fluid inlet, yellow for symmetry, and black for wall.

Figure 6.9: Shape development over 100 iterations, taken for path D. The shapes do not show sharp edges for iteration 5. Difference of shapes in the flow direction can be seen starting from iteration 10, and is more pronounced with more iterations. Iteration 100 represents the final optimized case.

that the whole array should have the same shape, shapes from iteration 25 or 50 can be employed with an increase of 1.9% and 3.6% of heat transfer and -2.6% and -7.1% pressure drop reduction, respectively. For the best performance, the final optimized geometry (iteration 100) can be used, resulting in 6.4% increase of heat transfer and 18.5% decrease in pressure drop. To conclude, the decision maker can choose different shapes according to his requirements and limitations by looking at Figure 6.4. Using this optimization procedure, a vast choice of shapes can be obtained as well as its performance, that can assist the decision maker in the selection process.

Figure 6.10: Typical problem of the deformed mesh (top). Note that the mesh elements near the indentations are highly stretched, leading to high aspect ratio elements. This problem is solved by the remeshing process (bottom) to make more uniformly shaped elements with low aspect ratio.

6.3.2 Remeshing

The final optimized shapes obtained in Chapter 6.4.1 undergo a large number of design iterations. Thus, the mesh quality decreases considerably, which necessitates a remeshing and recomputation of the flow solution. Typical grid element of the deformed mesh and the remeshing results are compared in Figure 6.10. To confirm the computed heat transfer and pressure drop of the final optimized geometry, a remeshing and recomputation of the flow state are performed for each of these geometries. The results are presented in Table 6.2.

By the remeshing, it is confirmed that the end solutions from the adjoint optimization procedure are constantly within 5% difference to the remeshed results for all optimized geometries. Hence the graphs in Figure 6.3 and Figure 6.4 still hold. For a better certainty, the mesh adaptation or automatic remeshing could be implemented for future work.

6.3.3 Cylinder array optimization: effect of crossing path

Based on Chapter 5, the study is extended by using various weight factors while setting the pressure drop step size as a relative percentage to the pressure drop of the previous design iteration. The utilization of the relative percentage is intended to advance the optimization procedure with more design iterations. As can be seen in Chapter 6.4.1, the lower pressure drop absolute value of the new geometry is preventing the optimization cycle to run further after a large number of

Table 6.2: Results of remeshing compared to the mesh deformation obtained from adjoint optimization procedure: heat transfer, pressure drop, minimum orthogonal ratio, and maximum aspect ratio.

Shape	Deformed mesh					Remesh				
	HT (W)	dP (Pa)	No. of elements	Min. ortho	Max. aspect	HT (W)	dP (Pa)	No. of elements	Min. ortho	Max. aspects
A	-1.498	0.504	34310	9.9E-04	9.7E+01	-1.497	0.483	22908	0.240	11.92
B	-1.525	0.464	34310	6.0E-04	1.6E+02	-1.519	0.464	242629	0.137	15.64
C	-1.523	0.437	34310	$\ll 1E-05$	2.2E+02	-1.514	0.441	27494	0.166	18.34
D	-1.471	0.377	34310	$\ll 1E-05$	6.6E+02	-1.459	0.378	29797	0.186	15.87
E	-1.394	0.325	34310	$\ll 1E-05$	9.1E+01	-1.393	0.325	32413	0.159	12.01
F	-0.180	0.017	34310	3.1E-03	5.3E+01	-0.181	0.017	33053	0.208	6.71
G	-1.469	0.134	37836	3.9E-04	5.6E+01	-1.460	0.135	31262	0.194	15.82
H	-1.396	0.127	37836	6.0E-04	1.2E+02	-1.396	0.128	33164	0.297	6.40
I	-1.377	0.123	37836	$\ll 1E-05$	3.7E+02	-1.372	0.126	33820	0.291	9.18
Initial geometry										
Cylinder	-1.382	0.465	34310	2.9E-01	6.7E+00					
Ellipse	-1.337	0.147	37836	4.4E-01	8.4E+00					

design iterations. Another reason for this choice of step size is due to the nonlinear behavior of the paths. The constant objective step sizes in Chapter 6.4.1 is chosen to better predict the location of the data points for the final optimized geometry in the objective space by assuming a linear behavior for the path. However, it is found that this is not the case as the paths in Figure 6.3 develop nonlinearly. Hence, using a relative percentage for pressure drop will add more nonlinearity to the path behavior and its effects on the path is investigated. Thus, for the work in this subchapter, the step size of pressure drop is set as a relative fraction of the pressure drop of the previous geometry, while the step size of the heat transfer is kept as an absolute value throughout the optimization cycle. Figure 6.11 depicts the paths resulting from various weight factors.

Using this setting, some paths are intersecting, resulting in two geometries that have the same performance. It is shown in Figure 6.11 that despite having the same initial geometry, the final optimized geometry is dependent on the path it undergoes. Point 1, 2, and 3 show the different geometries for each crossing paths, suggesting that there is not a unique solution for different weight factors. Although point 1 and point 2 give similar shapes, however these shapes are not exactly the same. For point 3, the difference is clearly seen.

Using this domain, it can be concluded that five cylinders in a row are not sufficient to perform adjoint optimization procedure for an array of pins. Clearly the effect of the bounding box can be seen on the first and the last cylinder, where the front and the rear part tend to form

Figure 6.11: Cylinder optimization using Domain $D3$. Markers placed for the first design iteration, and afterwards for every 10 design iterations. Effect of the crossing paths can be seen on the shapes on the right.

a straight profile. This profile is obtained due to the mesh movement towards the left and right side of the bounding box, hence leading to high density elements compressed between the cylinder surface and the bounding box. To improve this study, more cylinders are added in the flow direction, as shown in Chapter 6.4.1. It is concluded that ideally, using seven cylinders in a row is sufficient to obtain a recursive pattern of the pin shape. Note that the effect of the left and right boundary of the bounding box is still visible on the first and the last cylinder in Chapter 6.4.1 even though the indentations is present.

6.3.4 Effect of different domain size and symmetry boundary condition

The effect of increasing the domain size in both x - and y -direction is studied in this subchapter. The domain size refers to the number of cylinders in an array. To the author's knowledge, no study about the number of cylinders that is sufficient for the adjoint optimization is reported in literature. The number of cylinders is critical to the adjoint optimization process in ANSYS Fluent due to the utilization of the bounding box. The boundary of the box limits the movement of the mesh points, therefore it is necessary to choose a number of cylinders such that the effect of the flow direction within an array of cylinders can be captured. This study aims to capture the different shapes within an array subject to the temperature difference in the flow direction. Furthermore, this study is useful to find the smallest domain

Figure 6.12: Size comparison of Domain $D1$ and the 18 times larger bounding box (left, for Domain $D1 - 2$, $D1 - 3$, $D1 - 4$) and the three times larger bounding box (right, Domain $D1 - 5$). The control points are distributed equidistantly within the bounding box.

or array size that can be used for ANSYS Fluent adjoint optimization to reduce the computational time. Therefore, to study the domain in the x -direction, Domain $D1$, $D3$, and $D4$ are used where the effects of using five, six, and seven rows of half-cylinders are observed. To study the domain size in the y -direction, Domains $D1 - 1$ and $D5$ are used. The results are presented in the following subsection.

6.3.4.1 Domain size in the x -direction

Two sizes of bounding box are used in this subchapter: three times larger and 18 times larger bounding box (Figure 6.12). This choice of bounding box size is due to the previous problem with the indentation (see Chapter 5), thus enlarging the box in the y -direction is tried as a solution.

Figure 6.13 shows the result of using six and seven half-cylinders to represent the array. It should be noted that these results are obtained using bounding box that is 18 times larger in the y -direction than the domain size. From the results, it can be seen that the indentations are well eliminated. Contrary to the results in 6.4.1, no recurring shapes emerge from the simulations. The front and rear cylinders of both cases show an almost straight profile, suggesting that the effect of the left and right boundary of the bounding box is still limiting the deformation.

From the aforementioned results, it is concluded that six and seven rows of cylinder in the x -direction may not be sufficient to represent the array. However, changing the size of the bounding box can lead to a different conclusion and the results are shown in Figure 6.14. For the Domain $D4 - 2$, using three times larger bounding box results in a heart-shaped pattern similar to the results in 6.4.1 (Figure 6.14 left). Thus, six rows of cylinders are sufficient for this size of the bounding

Figure 6.13: Comparison of the final optimized geometry between the six half-cylinders (Domain $D4 - 1$, left) and the seven half-cylinders (Domain $D1 - 2$, right). Both simulations are run using 18 times larger bounding box, 20×20 control points in the x - and y -direction, and $-1e - 03W$ and $-1e - 03Pa$ step size for heat transfer and pressure drop optimization. Indentations are well eliminated.

Figure 6.14: Left: Final optimized geometry for Domain $D4 - 2$, run with three times larger bounding box and 20×20 control points. A recurring shape can be seen here. Right: Final optimized geometry for Domain $D1 - 3$, run with 18 times larger bounding box and 20×60 control points. Similarly to Figure 6.13(right), no recurring shape is obtained, indicating that seven rows of cylinder might not be sufficient to portray the array with this size of bounding box.

box. On the other hand, the larger the bounding box, more rows of cylinders in the flow direction is needed due to the strong stretching in the y -direction. For the 18 times larger bounding box, it is highly likely that seven rows of cylinder are sufficient to obtain a patterned shape. Changing the number of control points from 20×20 (in the x - and y -direction) to 20×60 is also not sufficient to portray the array, as shown in Figure 6.13(right) and Figure 6.14(right). Therefore, it was concluded that the number of cylinder rows depends on the size of the bounding box to sufficiently portray the array. Generally, six rows of cylinder in the direction of the flow is sufficient to represent the cylinder array, considering that the bounding box size is three times the domain size in the y -direction. With larger bounding box, more numbers of rows are needed.

6.3.4.2 Domain size in the y -direction

The Domain $D1 - 1$ is multiplied six times in the y -direction to form the Domain $D5$. A tapered outlet is used to prevent the back flow. The aim of this study is to observe the effect of the symmetry boundary

conditions on the half-cylinders at the top and at the bottom of the domain. Moreover, the shapes of the cylinders in the interior of the domain are also sought, as it is suspected that there will be no indentation problem for these cylinders. The number of control points in the x - and y -directions is chosen such that a constant control point distribution is maintained between the two domains, hence 20×5 and 20×30 for the Domain $D1 - 1$ and $D5$, consecutively. Both domains used the slightly larger bounding box with a 0.2 mm clearance each at the top and at the bottom of the domain.

The optimization results for the Domain $D5$ show that the indentations occur in the upper and lower boundaries only (Figure 6.15). This is in accordance with earlier observation in Chapter 6.4.1 with a slightly larger bounding box (Domain $D1 - 1$), where the delay of movement also occurs in the symmetry boundary lines. As shown in Figure 6.15, the shapes at the interior do not have any indentations. With more design iterations, it can be observed that the pins are cluttered into four regions: inlet, outlet, upper and lower sides. The grouping of the pins may be influenced by the upper and lower symmetry, as well as the left and the right side of the bounding box. The pressure drop is set to have more weight than the heat transfer, hence the end geometry is deformed such that the fluid channel is enlarged, resulting in an X-shaped fluid channel in the middle of the domain that clusters the pins into four regions.

It should be emphasized that the bounding box will always be a limiting factor in this optimization procedure, therefore one cannot exactly simulate a real geometry of the heat exchanger due to the limitation of the symmetry boundary condition. Moreover, as long as the mesh is deformed using the freeform deformation method involving a certain bounding box, the optimization results will not represent the real object. Since the bounding box will limit the movement of the mesh point close to its boundaries, the constrained movement will always be visible within the computational domain. Thus, obtaining a recursive shape for the current geometry can be challenging, and one should probably introduce some constraints to the movement of the mesh points, e.g. by keeping distance of the center of gravity of each pin to be equal. Unfortunately, this feature is not available in the current optimization platform and could be added for future improvement.

To eliminate the indentation, one can (1) enlarge the bounding box or (2) enlarge the computational domain such that the effect of the bounding box boundaries will be minimized at the interior. As discussed above, enlarging the bounding box up to 18 times larger leads to some aspects that needs to be considered. First, most of the control points will be distributed outside of the computational domain. It should be taken into account that these control points have contributions to the total deformation of each mesh points. On the other hand, if one wants to

Figure 6.15: Adjoint optimization results of Domain $D5$. A slightly larger bounding box is used with 20×30 control points in x - and y -direction. Taken for $-1e-03W$ and $-1e-02$ Pa step size.

enlarge the domain and take the interior shapes as the final optimized geometry, it should be noted that the shapes near the boundaries may have a high impact on the overall performance of the whole domain. Therefore, it may occur that the interior pins do not necessarily perform as good as the pins near the boundaries. Second, enlarging the domain up to six times does not give a recursive shapes as shown in Figure 6.15 but it results in the clustering of the pins into four regions due to the strong effect of the four boundaries of the bounding box instead. Applying geometrical constraints in ANSYS Fluent to limit the movement of the mesh points can be considered as an alternative and this task is left for future work.

6.3.5 Bounding box and control points

The correlation between the bounding box size and the control point distribution is further studied. This study is intended only for the application of adjoint method in ANSYS Fluent, in which a bounding box is required for the mesh morphing process.

Figure 6.16: Results of the adjoint optimization of the Domain $D1$ for different box sizes. The number of control points in the y -direction is changed according to the length of the bounding box in the y -direction to maintain the same distribution of the control points within the bounding box.

Seven rows of half-cylinders are used in this subchapter. First, the size of the bounding box is varied in the y -direction while keeping the control point distribution constant. Using the sizes depicted in Figure 6.12, the number of control points in the y -direction is chosen while keeping the same control point distribution as Domain $D1 - 1$ (20x5 control points). For the 18 times larger box, number of control points in the y -direction is multiplied by 18, resulting in Domain $D1 - 4$ with 20x90 control points. Similarly, for the three times larger box, the number of control points in the y -direction is 15, resulting in Domain $D1 - 5$. With the three variations of bounding box sizes, the adjoint optimization procedure is run for the same objective target: $1e - 03W$ and $1e - 03Pa$ per design iteration.

Figure 6.16 shows the results of the adjoint optimization for the three cases. For the 18 times larger box, most of the control points are located outside the domain. The contribution of these control points to the mesh deformation can be seen strongly on the final optimized shape. The 18 times larger box results in a less indented cylinders, while the slightly larger and three times larger box tend to result in similar shapes. In terms of performance, lower pressure drop can be achieved using the 18 times larger box. The case with three times larger box stopped at the 62nd iteration due to the occurrence of negative cells when deforming the mesh, indicating a too large of a step size. On the contrary, the other two cases can be run further while keep increasing the performance. This indicates that the three cases converge towards different local optima. This is also proven by the different final geometries obtained at the end of the optimization procedure.

Secondly, the variation of the control point distribution is studied while maintaining the same size of the box. 20x20 (Domain $D1 - 2$), 20x60 (Domain $D1 - 3$), and 20x90 (Domain $D1 - 4$) control points are used and the final optimized geometry as well as the performance are

Figure 6.17: Results of the adjoint optimization of the Domain $D1$ for different control point distributions. The size of the bounding box is maintained to be constant for the three simulation cases while the number of control points in the y -direction is varied.

compared. As expected, the 20×20 control point is the most limiting case. Due to the large spacing between control points and the relatively small deformation allowed for each control point, this case does not lead to a large deformation of the domain. Moreover, the simulation stops automatically at the 42^{nd} iteration due to the generation of negative cells during the mesh morphing process.

The effect of the number of control points to the performance as well as the final optimized geometry is shown in Figure 6.17. It is observed that there is not a significant difference in terms of performance between using 20×20 control points or 20×60 . In terms of the final shapes, more control points lead to later stop of the simulation and consequently more deformations. Since no mesh refinement is employed, it is unclear whether both are deforming towards the same optimum point. However, looking at the final geometries for CP 20×60 and 20×90 that are quite different, it is highly likely that the optimizer aims for different optimum points, as different number of control points represents different optimization case.

Furthermore, it is concluded that the effect of control point distribution is less significant than the effect of changing the box size. As can be seen in Figure 6.17, the three cases have the same gradient of the performance curve. The only difference is the point where the simulation stops, which indicates that each of these cases improve towards different local optima. The three cases are all stopped due to a too large of a step size, hence no further improvement could be obtained. Furthermore, the final shapes of the three cases look similar, especially the 20×60 and 20×90 case. This means that changing the number of control points in the y -direction for such a large box does not give significant difference. Compared to Figure 6.16, the difference caused by changing the box size is more pronounced.

6.4 SUMMARY

An automatic adjoint optimization procedure is performed based on the parameter study of arrays of circular cylinders. The adjoint optimization procedure is proven to be able to achieve a better performance beyond the conventional Pareto front for circular cylinder array and ellipse array. Both arrays show the same tendency towards a typical final optimized geometry for weighted heat transfer or pressure drop. The final optimized geometries are remeshed and the flow state is recomputed to confirm the heat transfer and pressure drop obtained from the adjoint optimization procedure. The results show that the differences are within 4% deviation, thus the adjoint optimization procedure can achieve a reliable flow state at the end of the procedure despite a poor mesh quality.

Various improvements of heat transfer and pressure drop based on the weighting factors can be achieved using this procedure. One example is the case C of the cylinder array, where the heat transfer is improved 10% and the pressure drop is reduced 6% beyond the conventional Pareto front. Furthermore, the ellipse optimization can also achieve 8% reduction of pressure drop and 15% increase of heat transfer relative to the ellipse initial geometry (path I). Compared to the initial cylinder geometry, this optimized shape has a better pressure drop but 10% less heat transfer as a penalty. These comparisons of the objectives can be seen in the objective space plot. Using this plot, one could choose a suitable design in terms of heat transfer and pressure drop according to the respective requirements.

Furthermore, the effects of crossing paths in the objective space to the geometries are studied. It is found that there is no unique solution for the same starting initial geometry, as each case depends on the path undergone by the optimized geometry. From this study, it is also revealed that five cylinders in a row is not sufficient to represent an optimization case for a cylinder array, as the effect of the bounding box limitation can be seen on the first and the last cylinder clearly. Thus, it is suggested that at least six rows of cylinders should be the minimum requirement for optimizing a cylinder array using ANSYS Fluent adjoint shape optimization procedure.

It should be noted that simulating a domain using symmetry boundary condition leads to a different optimum point than the real optimum of the real full domain. The computational domain should be looked at as a whole, instead of for each cylinder. The contribution of the cylinders near the boundaries of the bounding box could be crucial in the performance of the whole domain. Thus, the shapes in the middle of the computational domain may lead to a different performance than what is expected by the user based on the performance of the whole domain. Moreover, changing the number of control points, domain size,

bounding box size, or weight factor leads to a different optimization case, hence different final geometry. These additional parameters (outside of the geometrical parameter of the array) should be taken into consideration when performing this adjoint optimization procedure.

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Part IV

3D ARRAY

In the fourth part of the thesis, studies involving three-dimensional model of an array of circular cylinders are presented.

3D MULTI-OBJECTIVE OPTIMIZATION OF CYLINDER ARRAY WITH CONJUGATE HEAT TRANSFER

Two-dimensional study presented in Chapter 6 leads to the development of a more complex three-dimensional model of an array of cylinders. This model is used for the adjoint shape optimization, however the procedure cannot successfully produce a shape that improves both objectives. In this chapter, the investigation of the failure of the adjoint procedure is presented. The root cause of the failure is sought and further recommendation is given for further studies.

ABSTRACT A 3D model of an array of circular cylinders is realized. The conjugate heat transfer with both periodic and symmetry boundary conditions are incorporated in the model. The laminar $Re_D = 100$ flow is simulated and the adjoint optimization procedure is performed on this model to improve the heat transfer and the drag force. However, the adjoint optimization procedure does not result in an improved shape and the root cause of the failure is investigated. The failed optimization case is compared with the successful case in Chapter 4 in terms of the initial steps conducted before the mesh morphing process. The step sizes study is done for the multi-objective optimization and the results are presented in a graph to find the optimization window of opportunity. Three regions are identified in the graph: possible mesh morphing region, too large step size region, and the no deformation region. Furthermore, the analysis on the expected change provided by the optimizer is presented in this chapter. This analysis gives an indication whether the mesh morphing will likely succeed in producing a shape that can improve both objectives or not. Compared with the successful optimization case in Chapter 4, it is found that the optimizer fails to predict a correct expected change, thus leading to the nonoptimized shape. Possible cause of this failure is the periodic boundary condition, however this case needs further research to confirm the real cause of the problem.

7.1 INTRODUCTION

The flow around an array of cylinders has been a subject of extensive study due to its application. In mechanical appliances, such as heat exchangers, the cylinder array is generally used as an additional surface to maximize the heat transfer per m^3 . The penalty for this increase in heat transfer is an increased pressure drop, thus a stronger driver of the flow

is needed. Thus, balancing the heat transfer and the system's pressure drop becomes one of the challenges in heat exchanger optimization.

Previous works regarding cylinder arrays can be found in [1, 2, 3]. However, all these works are focused on the mechanics of flow around a cylinder, in a staggered or in-line arrangement. A study for cylinder and ellipse array done by Horvat and Mavko [3] found that more complex physical behavior was observed from their unsteady simulations. The spanwise motion becomes important as the flow regime changes from laminar to turbulent. This observation is consistent with the results in Chapter 3 with the single cylinder. In the previous chapters, two-dimensional simulations for the cylinder array has been performed, however as the spanwise motion is important, a three-dimensional optimization is interesting to investigate. Nevertheless, considering the cost of performing unsteady simulation that is computationally expensive and the unsteady adjoint that is not available yet in ANSYS Fluent platform, a steady three-dimensional optimization is then performed for the cylinder array. Further justification was made by the fact that the Reynolds number, although it is within the region of unsteady flow, is relatively low and is damped by the cylinder array such that a steady flow is developed throughout the array. Only the last row of cylinders downstream produce the von Kármán vortex shedding. Therefore, in the current chapter, a periodic boundary condition is used to model the cylinders in the interior of the array which do not generate the von Kármán vortex.

To the authors' knowledge, no study of shape optimization for a cylinder array using a three-dimensional, conjugate heat transfer model has been performed. Thus, it is interesting to see the shapes resulting from the adjoint optimization procedure for the current cylinder array model. However, some challenges arise during the optimization process that lead to a detailed study about the multi-objective optimization. As the optimizer failed to improve both objectives, it is therefore important to find the root cause of this problem.

To investigate this, a step size study is performed for both objectives and the nature of the optimizer's prediction for the improved objectives are analyzed. Furthermore, the currently failed optimization for is compared with the successful optimization case presented in Chapter 4. Note that both cases use the conjugate heat transfer model, however there are differences that are worth mentioning: (1) the case in Chapter 4 uses $Re_D = 10$ while the current case use $Re_D = 100$, (2) the case in Chapter 4 uses a full length single cylinder while the current case uses a half-length cylinder array with symmetry boundary condition, and (3) the current case uses the periodic boundary condition at the inlet and outlet while the case is Chapter 4 does not. Despite these differences, the parameter comparison of the current case and Chapter 4 case lies in the optimizer's performance that can be seen clearly even for different

cases. In this chapter, the explanation on the possible cause of failure is presented together with recommendation for further studies.

7.2 METHODOLOGY

The three-dimensional domain is shown in Figure 7.1. A flow with Reynolds 100 and a temperature of 289.16K is imposed at the inlet. The inlet and the outlet of the domain are made as a periodic boundary condition. This type of boundary condition will be explained further in this chapter. The cylinders are mounted to a 3mm thick base plate made of aluminum with properties listed in Chapter 1. At the bottom of the base plate, a constant temperature of 288.16K is imposed. The side walls in between the cylinders are set to be symmetric, as well as the top plane at the tip of the cylinders.

Figure 7.1: Computational domain and boundary conditions. The number 1, 2, and 3 represents the number of the cylinders and are used from this point onward. Constant fluid and solid properties are used for this computational domain.

The definition of the streamwise-periodic pressure is given in Equation 7.1.

$$\Delta p = p(\vec{r}) - p(\vec{r} + \vec{L}) = p(\vec{r} + \vec{L}) - p(\vec{r} + 2\vec{L}) \quad (7.1)$$

where $\vec{r}$ is the position vector and $\vec{L}$ is the periodic length vector of the domain considered. Thus, the pressure drop between modules is

periodic. In the currently used pressure-based solver, the local pressure gradient can be decomposed into two parts as shown in Equation 7.2.

$$\nabla p(\vec{r}) = \beta \frac{\vec{L}}{|\vec{L}|} + \nabla \tilde{p}(\vec{r}) \quad (7.2)$$

The first term on the right hand side of the equation represents the gradient of a linearly-varying component, while the second term is the gradient of a periodic component. The linearly varying component of the pressure results in a force acting on the fluid in the momentum equations. Since the periodic boundary condition in ANSYS Fluent is set by specifying the mass flow rate at the inlet, the value of β must be iterated until the mass flow rate is equal to the one specified [7].

In simulating a periodic heat transfer, only the scaled temperature is considered periodic, while the absolute temperature is not periodic [7]. The scaled temperature θ is defined as follows:

$$\theta = \frac{(T - T_{wall})}{(T_{bulk,inlet} - T_{wall})} \quad (7.3)$$

where the inlet bulk temperature is defined as:

$$T_{bulk,inlet} = \frac{\int_A T \rho \vec{v} d\vec{A}}{\int_A \rho \vec{v} d\vec{A}} \quad (7.4)$$

For the heat flux iteration, the calculation between Equation 7.5 and 7.6 should converge:

$$\frac{T(\vec{r} + \vec{L}) - T(\vec{r})}{L} = \frac{T(\vec{r} + 2\vec{L}) - T(\vec{r} + \vec{L})}{L} = \sigma \quad (7.5)$$

$$\sigma = \frac{Q}{\dot{m} C_p L} = \frac{T_{bulk,outlet} - T_{bulk,inlet}}{L} \quad (7.6)$$

In using the periodic boundary condition for the heat transfer calculation, there are limitations in ANSYS Fluent, as listed below:

1. The solid region cannot be in contact with the periodic boundary condition of the fluid.
2. Only constant thermal properties are allowed.
3. When a constant temperature is imposed to the wall, the viscous heating effect and volumetric heat sources are not included in the solution.

These limitations result in the constant temperature boundary condition specified in Figure 7.1 and the constant thermal properties used throughout the simulation.

7.3 RESULTS

7.3.1 Laminar Flow

The results of the adjoint optimization procedure for $Re = 100$ are shown in this subchapter. Firstly, the shape sensitivities are obtained from the adjoint calculation for both heat transfer and drag force. The results are depicted in Figure 7.2 and Figure 7.3, respectively.

The shape sensitivity vector for the heat transfer optimization shows that all arrows are pointing outwards of the solid domain, as expected for increasing the heat transfer surface. The highest magnitude occurs at the 180° angle of the second cylinder. This result is in accordance with the velocity contour of the initial geometry (Figure 7.4a). When looking at the temperature contour plot (Figure 7.4b), the gradual decrease in temperature downstream do not significantly affect the sensitivity vectors of the heat transfer optimization.

For the drag minimization, the sensitivity vector plot shows the inwards direction into the solid domain (Figure 7.3), corresponding to the attempt of the optimizer to minimize the surface area. The high magnitude vectors at around $\theta = 45^\circ$ and $\theta = 135^\circ$ correspond well with the velocity contour plot in Figure 7.4. The blockage caused by the staggered arrangement of the cylinders results in two high-velocity regions. On the other hand, the temperature contour plot shows highest temperature around the front stagnation point of the second cylinder, as this region is closest to the heat source. However, taking into account of the velocity contour plot, it is reasonable that the highest heat transfer could occur around the area ranging from the front stagnation point towards $\theta = 135^\circ$.

Looking at the magnitude of the sensitivity vectors of both objectives, it can be seen that the heat transfer holds more weight by two order of magnitudes higher than the drag sensitivity. Furthermore, looking at the location of the maximum sensitivity vectors for both observable ($\theta = 180^\circ$ for heat transfer and $\theta = 45^\circ$ for drag), it is highly possible that the optimization procedure can result in an optimized shape by modifying the shape at these locations. However, the current trial and error determination of the weight factors cannot provide a successful optimization, explained as follows.

As presented in Figure 2.2, the mesh morphing procedure consists of four steps: setting up the step sizes for both objectives, calculate the expected changes, modify the shape, and recomputation of the flow. After getting the sensitivity information, the step sizes are determined to set the weight factors. Thus, the choice of these step sizes is crucial to the optimization procedure [8]. In ANSYS Fluent mesh morphing process, too large a step size could result in negative cell volume, i.e. the mesh is morphed such that the new mesh cell has an extremely

Figure 7.2: Shape sensitivity magnitude for the heat transfer maximization: (a) maximum sensitivity obtained at the top of the second cylinder, (b) shape sensitivity magnitude around the front stagnation point, and (c) top view of the shape sensitivity magnitude, plotted for the whole cylinder. Note that all arrows are pointing outwards of the solid domain.

Figure 7.3: Shape sensitivity magnitude for the drag force minimization: (a) maximum sensitivity obtained at around 45° angle, (b) top view of the shape sensitivity magnitude, plotted for the whole cylinder. Note that all arrows are pointing inwards of the solid domain.

high skewness. The negative cells could lead to convergence problems and inconsistency at the solid-fluid interface for the conjugate heat transfer model. On the other hand, too small a step size will force the mesh morpher to retain the same geometry, i.e. no deformation occurs. Thus, the objective step sizes should be chosen within a certain window in which (1) the mesh morphing process deforms the mesh elements, and (2) the deformation results in an improvement of both objectives. To obtain such step sizes, numerous trial and errors should be done first. An example of the result of the trial and error to find the possible window is presented in Figure 7.4.

Figure 7.4 presents three possible regions that indicate the possible mesh morphing process. The deformed region indicate that a mesh morphing is possible to be performed, whereas the other two regions

Figure 7.4: Step size study to find the possible window of opportunity for the multi-objective optimization, plotted for the failed cylinder array case. Three regions are visible: the deformed region (circle), negative cells region due to too large step size (dot), and no deformation region due to too small step size (cross).

(the too large deformation and the no deformation regions) refer to the failed mesh morphing process. The determination whether the mesh morphing results in too large deformation, too small deformation, or a good deformation can be seen by looking at the so-called *expected change*. The expected change is the computed change of objectives obtained after setting up the step sizes and before morphing the mesh (see the workflow in Figure 2.2). This way, the user has an information beforehand whether the new geometry will likely result in an improvement or not. The expected change listed in Table 7.1 are then confirmed by morphing the mesh. If the deformation is too large, the mesher will give a warning of *negative cells*. On the other hand, when there is no deformation, the user can expect this by looking at the values of the expected change: its order of magnitudes are small (i.e. $7E - 23N$).

Since the shape sensitivity vector magnitude for the heat transfer has more weight than the one of the drag force, the heat transfer step size is the limiting objective. For example, in Figure 7.4, the heat transfer step size should be around $-1e - 05$ W to ensure that the mesh is morphed. As can be seen, the step size of $-1e - 05$ W can be combined with a wide range of drag force step sizes, from $-1e - 06$ to $-1e - 10$ N. Choosing a step size larger than $-1e - 04$ W, for example, results in

too large deformation. On the other hand, choosing a step size smaller than $-1E-05$ W results in no deformation. Other limiting factor is the drag force step size: a step size larger than $-5E-06$ N will result in a too large deformation. The data points plotted in Figure 7.4 are listed in Table 7.1.

After obtaining Figure 7.4 and Table 7.1, the user can now choose the step sizes and morph the mesh. By looking at the expected change, the user should choose the ones that give larger negative values than the initial value of the objectives. Note that the drag and heat transfer values for the initial geometry are, respectively, $1.81E-05$ N and $-1.91E-02$ W. From Table 7.1, it can be seen that there are several possibilities for improvement of both objectives, e.g. data number 22, 27, and 32. The mesh elements are then morphed according to these data and the flow is recomputed to confirm whether the new design results in improved objectives or not. The results of these flow recomputation is shown in Table 7.2, with additional data points.

The results of the flow recomputation in Table 7.2 show that none of the chosen step sizes lead to improvement of both objectives, only the drag force is improved instead. Evidently the adjoint optimization procedure in ANSYS Fluent could give: (1) a faulty prediction of the expected change (i.e. expected change is not equal to the step sizes specified), that leads to (2) no improvement of the objectives. Looking at the trend of heat transfer's expected change with the change of the step sizes, it seems that giving smaller step size to the drag force will increase the weight of heat transfer, thus increasing the chance of the heat transfer to improve. As can be seen by the last data point, the drag step size was chosen as $-1E-15$ N, however as the drag step size is approaching zero, the heat transfer recomputation does not result in a large enough change to surpass the initial value. In order to improve the heat transfer, a single objective optimization may be the only option and therefore the drag will be deteriorated. This conclusion seems to be contradictory with the sensitivity vectors, i.e. the location of the maximum sensitivities of both objectives are not overlapping, nor the magnitudes of both objectives the same, hence there should be a possible design change that improves both objectives. Note that the results in Table 7.2 is achieved using the computed sensitivities resulting from the adjoint solver (Figure 7.2 and Figure 7.3). It was concluded that the adjoint solver itself is working properly, however the optimizer might be erroneous. To check this, this non-successful optimization case is compared to the successful one of the single cylinder in Chapter 4 to find out the possible reasons.

Firstly, the same method is employed to construct Figure 7.4 for the single cylinder case. The results are depicted in Figure 7.5 for this case. Similar to Figure 7.4, three regions of mesh deformation can be seen in this graph: the too large deformation, no deformation, and the

Figure 7.5: Step size study to find the possible window of opportunity for the multi-objective optimization of the successful single cylinder case (Chapter 4). Similar to the failed case, three regions are visible in this graph: the deformed region (circle), negative cells region due to too large step size (dot), and no deformation region due to too small step size (cross).

deformed region. The data points are listed in Table 7.3. From this table, we can see a clear distinction of the expected change values compared to Table 7.1 and Table 7.2.

While the values of the expected change in Table 7.1 and Table 7.2 are diverse, in Table 7.3 these values are exactly the same as the ones specified in the step sizes column, regardless of the region whether it is deformed or negative cells. Only the no deformation data points show different values than the values specified in the step sizes column, with a significantly small order of magnitude. Of these data points, no flow recomputation was performed, except for data number 7 which results indeed in improved drag and heat transfer (presented in Chapter 4).

It is clear that for the cylinder array case, the optimizer is not working properly, hence resulting in a faulty expected change despite its correct adjoint solutions. The adjoint solutions seem to be correct, as can be seen by the direction of the shape sensitivity vectors in Figure 7.2 and Figure 7.3. Other possible reasons of failure are: (1) the problematic symmetry boundary conditions, (2) the failure of the conjugate heat transfer model, and (3) the failure of the periodic boundary condition. Symmetry boundary conditions and conjugate heat transfer model are

both used in the Chapter 4 case, hence these reasons are eliminated since the adjoint optimization procedure works properly for this case. Thus other possible reason that could affect the faulty optimizer is the periodic boundary condition that is not used in Chapter 4. Up to this moment, it is not confirmed with ANSYS developers whether this is indeed true or not. We have confirmed that there are three factors that could make the prediction matches with the real change: (1) convergence of the flow and adjoint solution, (2) the deformation should be small to avoid nonlinear error, (3) the effect of changes in turbulence quantities [9] when the design approach the optimal state. We conclude that convergence is not the cause of the problem, as presented by the residual plots in Appendix A. The determination of the deformation is given by Figure 7.4 and small deformation can be chosen according to this figure. Thus, there is also a possibility that the flow is not fully laminar and that the current design is close to the optimal state. This problem is not pursued further in this thesis and remain a future work should the adjoint optimization be used for other three-dimensional cases with periodic heat transfer.

7.4 SUMMARY

A three-dimensional adjoint shape optimization is performed for an array of cylinders in at $Re_D = 100$. The adjoint optimization procedure failed to produce an optimized design, improving only the drag force instead of both objectives. The root cause of this failed optimization is investigated and this case is compared with the successful case of single cylinder optimization in Chapter 4. The difference can be seen in the expected values calculated by the optimizer: the successful case in Chapter 4 result in exactly the same value as the specified step sizes, contrary to the failed cylinder array case. Thus it is confirmed that the optimizer results in a faulty calculation that leads to the faulty mesh morphing and non-improved geometry.

Furthermore, a visualization of three regions of deformation is made for both cases to find out the possible range of step sizes that could result in a successful optimization. Similar plots are produced by both cases. The reason of the failure of the optimizer is not clear at the moment, however it is suspected that the periodic boundary condition is not implemented correctly as this boundary condition is not used for the successful case in Chapter 4. Aside from this reason, other possible causes are likely to be discovered with further studies. For the next step of this research, it is recommended to reconduct the current optimization by eliminating the periodic boundary condition to check the performance of the optimizer.

Table 7.1: Results of step size study for the cylinder array. Three types of mesh deformation is generated: too large deformation (negative cells), too small deformation, and deformed mesh.

No.	Step size		Expected change		Result
	Drag (N)	HT (W)	Drag (N)	HT (W)	
1	-1E-09	-1E-03	3.54E-05	-5.53E-04	Negative cells
2	-1E-05	-1E-04	3.53E-06	-5.53E-05	Negative cells
3	-1E-09	-1E-04	-6.33E-06	-5.29E-05	Negative cells
4	-6E-05	-6E-05	-5.71E-05	-1.85E-05	Negative cells
5	-5E-05	-5E-05	-4.76E-05	-1.54E-05	Negative cells
6	-1E-05	-5E-05	-8.10E-06	-2.52E-05	Negative cells
7	-1E-06	-5E-05	7.81E-07	-2.74E-05	Negative cells
8	-1E-07	-5E-05	1.67E-06	-2.76E-05	Negative cells
9	-1E-08	-5E-05	1.76E-06	-2.77E-05	Negative cells
10	-1E-09	-5E-05	1.77E-06	-2.77E-05	Negative cells
11	-1E-10	-5E-05	1.77E-06	-2.77E-05	Negative cells
12	-1E-06	-4E-05	-4.27E-07	-2.19E-05	Negative cells
13	-1E-06	-3E-05	7.38E-08	-1.63E-05	Negative cells
14	-5E-05	-1E-05	-4.90E-05	6.67E-06	Negative cells
15	-1E-05	-1E-05	-9.52E-06	-3.09E-06	Negative cells
16	-5E-06	-1E-05	-4.58E-06	-4.31E-06	Negative cells
17	-5E-05	-1E-06	-9.87E-05	2.38E-05	Negative cells
18	-1E-05	-1E-06	-9.84E-06	1.89E-06	Negative cells
19	-5E-05	-1E-07	-4.93E-05	1.21E-05	Negative cells
20	-1E-05	-1E-07	-9.86E-06	2.38E-06	Negative cells
21	-1E-05	-5E-06	-4.58E-06	-4.31E-06	Negative cells
22	-1E-06	-2E-05	-2.80E-07	-1.08E-05	Deformed
23	-1E-07	-2E-05	6.09E-07	-1.10E-05	Deformed
24	-1E-08	-2E-05	6.97E-07	-1.10E-05	Deformed
25	-1E-09	-2E-05	7.06E-07	-1.10E-05	Deformed
26	-1E-10	-2E-05	7.07E-07	-1.11E-05	Deformed
27	-1E-06	-1.5E-05	-4.57E-07	-8.05E-06	Deformed
28	-1E-07	-1.5E-05	4.32E-07	-8.27E-06	Deformed
29	-1E-08	-1.5E-05	5.21E-07	-8.29E-06	Deformed
30	-1E-09	-1.5E-05	5.29E-07	-8.29E-06	Deformed
31	-1E-10	-1.5E-05	5.30E-07	-8.29E-06	Deformed
32	-1E-06	-1E-05	-6.34E-07	-5.28E-06	Deformed
33	-1E-07	-1E-05	2.55E-07	-5.50E-06	Deformed
34	-1E-08	-1E-05	3.44E-07	-5.53E-06	Deformed
35	-1E-09	-1E-05	3.53E-07	-5.53E-06	Deformed
36	-1E-10	-1E-05	3.54E-07	-5.53E-06	Deformed
37	-1E-06	-5E-06	7.28E-23	1.78E-22	No deformation
38	-1E-07	-5E-06	7.28E-23	1.78E-22	No deformation
39	-1E-08	-5E-06	7.28E-23	1.78E-22	No deformation
40	-1E-09	-5E-06	7.28E-23	1.78E-22	No deformation
41	-1E-10	-5E-06	7.28E-23	1.78E-22	No deformation
42	-1E-06	-1E-06	7.28E-23	1.78E-22	No deformation
43	-1E-07	-1E-06	7.28E-23	1.78E-22	No deformation
44	-1E-08	-1E-06	7.28E-23	1.78E-22	No deformation
45	-1E-09	-1E-06	7.28E-23	1.78E-22	No deformation
46	-1E-10	-1E-06	7.28E-23	1.78E-22	No deformation

Table 7.2: Results of flow recomputation for the first design iteration of some data in Table 7.1. Note that the drag and heat transfer value of the initial design are, respectively, $1.8154E-05$ N and $-1.9066E-02$ W. None of the following data result in improvement of both objectives.

No.	Step size		Expected change		Iteration 01 flow recompute	
	Drag (N)	HT (W)	Drag (N)	HT (W)	Drag (N)	HT (W)
22	$-1E-06$	$-2E-05$	$-2.80E-07$	$-1.08E-05$	$1.7777E-05$	$-1.8761E-02$
27	$-1E-06$	$-1.5E-05$	$-4.57E-07$	$-8.05E-06$	$1.7702E-05$	$-1.8811E-02$
32	$-1E-06$	$-1E-05$	$-6.34E-07$	$-5.28E-06$	$1.7642E-05$	$-1.8854E-02$
	$-5E-07$	$-1E-05$	$-1.40E-07$	$-5.41E-06$	$1.7920E-05$	$-1.8919E-02$
	$-4E-07$	$-1E-05$	$-4.12E-08$	$-5.43E-06$	$1.7980E-05$	$-1.8931E-02$
	$-3E-07$	$-1E-05$	$5.75E-08$	$-5.46E-06$	$1.8040E-05$	$-1.8941E-02$
	$-2E-07$	$-1E-05$	$1.56E-07$	$-5.48E-06$	$1.8101E-05$	$-1.8952E-02$
33	$-1E-07$	$-1E-05$	$2.55E-07$	$-5.50E-06$	$1.8163E-05$	$-1.8961E-02$
35	$-1E-09$	$-1E-05$	$3.53E-07$	$-5.53E-06$	$1.8226E-05$	$-1.8970E-02$
	$-1E-15$	$-1E-05$	$3.54E-07$	$-5.53E-06$	$1.8227E-05$	$-1.8970E-02$

Table 7.3: Results of step size study for the single cylinder case (Chapter 4). The successful optimization presented in Chapter 4 is data number 7 with drag optimized from $8.87E - 07$ N to $8.71E - 07$ N and heat transfer from $-1.25E - 02$ W to $-1.25E - 02$ W.

No.	Step size		Expected change		Result
	Drag (N)	HT (W)	Drag (N)	HT (W)	
1	$-1E - 10$	$-1E - 02$	$-1E - 10$	$-1E - 02$	Negative cells
2	$-1E - 10$	$-1E - 03$	$-1E - 10$	$-1E - 03$	Negative cells
3	$-1E - 10$	$-1E - 04$	$-1E - 10$	$-1E - 04$	Negative cells
4	$-1E - 10$	$-9E - 05$	$-1E - 10$	$-9E - 05$	Deformed
5	$-1E - 09$	$-9E - 05$	$-1E - 09$	$-9E - 05$	Negative cells
6	$-5E - 09$	$-9E - 05$	$-5E - 09$	$-9E - 05$	Negative cells
7	$-1E - 08$	$-9E - 05$	$-1E - 08$	$-9E - 05$	Negative cells
8	$-1E - 07$	$-9E - 05$	$-1E - 07$	$-9E - 05$	Negative cells
9	$-1E - 10$	$-7E - 05$	$-1E - 10$	$-7E - 05$	Deformed
10	$-1E - 09$	$-7E - 05$	$-1E - 09$	$-7E - 05$	Deformed
11	$-5E - 09$	$-7E - 05$	$-5E - 09$	$-7E - 05$	Deformed
12	$-1E - 08$	$-7E - 05$	$-1E - 08$	$-7E - 05$	Negative cells
13	$-1E - 07$	$-7E - 05$	$-1E - 07$	$-7E - 05$	Negative cells
14	$-1E - 10$	$-5E - 05$	$-1E - 10$	$-5E - 05$	Deformed
15	$-1E - 09$	$-5E - 05$	$-1E - 09$	$-5E - 05$	Deformed
16	$-5E - 09$	$-5E - 05$	$-5E - 09$	$-5E - 05$	Deformed
17	$-1E - 08$	$-5E - 05$	$-1E - 08$	$-5E - 05$	Deformed
18	$-2E - 08$	$-5E - 05$	$-2E - 08$	$-5E - 05$	Negative cells
19	$-5E - 08$	$-5E - 05$	$-5E - 08$	$-5E - 05$	Negative cells
20	$-1E - 07$	$-5E - 05$	$-1E - 07$	$-5E - 05$	Negative cells
21	$-1E - 10$	$-2E - 05$	$-1E - 10$	$-2E - 05$	Deformed
22	$-1E - 09$	$-2E - 05$	$-1E - 09$	$-2E - 05$	Deformed
23	$-5E - 09$	$-2E - 05$	$-5E - 09$	$-2E - 05$	Deformed
24	$-1E - 08$	$-2E - 05$	$-1E - 08$	$-2E - 05$	Deformed
25	$-2E - 08$	$-2E - 05$	$-2E - 08$	$-2E - 05$	Deformed
26	$-5E - 08$	$-2E - 05$	$-5E - 08$	$-2E - 05$	Negative cells
27	$-1E - 10$	$-1E - 05$	$-1E - 10$	$-1E - 05$	Deformed
28	$-1E - 09$	$-1E - 05$	$-1E - 09$	$-1E - 05$	Deformed
29	$-5E - 09$	$-1E - 05$	$-5E - 09$	$-1E - 05$	Deformed
30	$-1E - 08$	$-1E - 05$	$-1E - 08$	$-1E - 05$	Deformed
31	$-2E - 08$	$-1E - 05$	$-2E - 08$	$-1E - 05$	Deformed
32	$-5E - 08$	$-1E - 05$	$-5E - 08$	$-1E - 05$	Negative cells
33	$-1E - 07$	$-1E - 05$	$-1E - 07$	$-1E - 05$	Negative cells
34	$-1E - 10$	$-9E - 06$	$-6E - 24$	$-1E - 21$	No deformation
35	$-1E - 09$	$-9E - 06$	$-6E - 24$	$-1E - 21$	No deformation
36	$-5E - 09$	$-9E - 06$	$-6E - 24$	$-1E - 21$	No deformation
37	$-1E - 08$	$-9E - 06$	$-6E - 24$	$-1E - 21$	No deformation
38	$-2E - 08$	$-9E - 06$	$-6E - 24$	$-1E - 21$	No deformation
39	$-1E - 10$	$-5E - 06$	$-6E - 24$	$-1E - 21$	No deformation
40	$-1E - 09$	$-5E - 06$	$-6E - 24$	$-1E - 21$	No deformation
41	$-1E - 08$	$-5E - 06$	$-6E - 24$	$-1E - 21$	No deformation
42	$-1E - 07$	$-5E - 06$	$-6E - 24$	$-1E - 21$	No deformation
43	$-1E - 10$	$-1E - 06$	$-6E - 24$	$-1E - 21$	No deformation
44	$-1E - 10$	$-1E - 07$	$-6E - 24$	$-1E - 21$	No deformation
45	$-1E - 10$	$-1E - 08$	$-6E - 24$	$-1E - 21$	No deformation
46	$-1E - 10$	$-1E - 09$	$-6E - 24$	$-1E - 21$	No deformation
47	$-1E - 10$	$-1E - 10$	$-6E - 24$	$-1E - 21$	No deformation

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Part V

DISCUSSION

CONCLUDING REMARKS

In this chapter, concluding remarks regarding the work in the preceding chapters are presented. While conclusions are drawn that are specifically for the propositions presented in the respective chapters, here the future outlooks are discussed and recommendations are given to solve the current limitations. This chapter is divided into several points of discussion as presented in the following passage.

- This work aims to find an improved design of the current Bosch heat exchanger in terms of heat transfer and pressure drop or drag force. In Chapters 4 to 7, several examples of improved geometries are presented. Every data point plotted in the objective space (i.e. in Figure 5.6a and 6.3) alludes to an improved geometry, enacting the graph with rich possible options of design improvements. The design options presented in the objective space provide the designer with ample selections to choose from, according to one's requirements and limitations. The flexibility and high number of design choices make the adjoint method a powerful tool for designers despite its limitations and imperfections.

Furthermore, as it is impossible to predetermine the end shape when using the freeform deformation for the mesh morphing, the adjoint method provides a good, targeted direction of improvement for the designer. Looking from a wider perspective, the adjoint method has a high potential to open new avenues for design improvements in the field of aerothermal system. Within the past ten years, shape optimization software, both the commercial and in-house software codes have shown rapid development. The advantage of the current commercial code relies in its wide applicability and simple user interface, leading to expedited production of new shapes. Users could experiment with the CFD parameters to arrive at a particular shape that will be best suited for the heat exchanger application. Combined with advanced manufacturing technology for complex shapes, this method will be applicable immediately in industry. This injects new innovations in the field of heat exchangers, with unlimited possibilities of new shapes for different applications.

- The application of the ANSYS adjoint procedure to the current Bosch heat exchanger geometry provides challenges in its modeling because the distinct parts of the heat exchanger have different flow conditions. For the low Reynolds flow, the adjoint shape

optimization can be applied directly using the laminar model. However, for the higher Reynolds flow, complications arise, leading to the DNS model described in Chapter 3 and the study of the adjoint optimization procedure in Chapter 7.

- In Chapter 3, the research question on the significance of the two- or three-dimensional simulation for low transition regime (transition in shear layer regime) is addressed by comparing the flow structure and the heat transfer properties resulting from both simulations. This flow regime occurs at the bottom part of the heat exchanger with $Re_D = 2000$. The results show that three-dimensional DNS is most suitable to model the transition in shear layer regime. However, the application of this model to the adjoint shape optimization procedure is unsuitable due to the high computational power to obtain the DNS solution. Additionally, the unsteady adjoint is not applicable yet in the current framework, hence this task is not discussed here. It is suggested that performing the ANSYS Fluent adjoint optimization procedure at the shear layer transition regime (or other transition regimes) is not recommended for the current framework.
- Another limitation that needs to be addressed is the computationally expensive issue of the trial and error procedure that needs to be conducted when finding the proper weight factors, which is contrary to the idea of using the adjoint method (Chapter 5 and 7). The intention of using the adjoint method is to reduce the time and effort in performing a manual trial and error procedure during the parameter variation in the design process. Compared to the conventional parameter variation (i.e. varying diameter, length, ellipticity), the adjoint method points the designer directly towards a certain direction of the design improvement. In the case of multi-objective optimization, the designer needs to set this direction by choosing the weight factors (or objective step sizes). However, as presented in Chapters 5 and 7, some trial and error is still needed to find out the proper weight factors that can result in optimizing both objectives. Based on the author's experience, the trial and error method of determining the weight factors takes a considerable amount of time, as one has to be able to find weight factors that satisfy both objectives and verify such a choice by rerunning a CFD solver. The methods suggested in Chapter 5 (by running a single-objective optimization first to get an idea on the correlation between the heat transfer and pressure drop) and Chapter 7 (by finding the window of opportunity as depicted in Figure 7.4 and Figure 7.5) are useful, however some flow computations still need to be conducted before the mesh morphing process can be done. Even though the cost of an adjoint

calculation is twice that of the CFD calculation, the total time needed for a complete shape optimization workflow becomes significantly larger (i.e. by taking into account the number of design iterations plus the pre-shape-change flow calculations).

Thus, it can be concluded that: (1) the adjoint gives more possibilities for shape improvement by having large possibilities of curved surfaces (compared to conventional trial and error of parameter variation), however (2) the trial and error procedure cannot be completely removed from the current workflow. Therefore it is recommended that an additional optimization algorithm is included within the ANSYS adjoint's framework to automatically determine the optimum weight factors. The implementation of this additional algorithm is outside the scope of this thesis and further research on weight factor optimization is needed.

- Another recommendation can be proposed about the symmetry boundary condition implemented in ANSYS Fluent. Since the most noticeable result of shape optimization is the indentation near the symmetry boundaries (see Chapters 5 and 6), it is therefore of paramount importance that the issue with the symmetry boundary condition within the adjoint routine is resolved. The current problem with indentation can be solved by manually modifying either (1) the shape sensitivity magnitude at the symmetry boundaries or (2) the mesh coordinate after the mesh morphing process. However, this manual intervention prevents the automation of the current ANSYS adjoint procedure. Modeling the whole geometry can be a solution in avoiding the use of the symmetry boundary condition, as demonstrated in Chapter 4, however this still provides a limitation on the size of the case that can be performed with the available computational power.
- The utilization of a bounding box for the mesh morphing process can lead to a few problems: (1) low mesh quality that requires remeshing after a considerable number of design iterations – Chapter 6; (2) effect of bounding box size and the number of control points – Chapter 6; (3) intersection with symmetry boundary condition – Chapter 5 and 6). It is therefore concluded that ANSYS Fluent adjoint optimization procedure should be used with great caution, in order to be able to produce a decent result for industrial applications. Resolving the symmetry boundary condition and bounding box issue will open a wider possibility for more complex geometries and further research.
- A solution for the low mesh quality after a large number of design iterations is to incorporate the remeshing into the automatic adjoint optimization procedure. A CAD-based parametrization

for the mesh morphing procedure such as the one used in [1, 2] can be adapted to the current automated optimization workflow. As the current parametrization method uses the freeform deformation (which is classified as CAD-free parametrization method, together with e.g. Lattice-based methods and Radial Basis Functions parametrization), it generates a problem when dealing with a large number of iterations as the mesh quality worsens. Although this type of parametrization method is frequently used over the past decades due to its straightforwardness, the most significant drawback of this method is that the morphed mesh exists only as a deformation field instead of a CAD geometry [2]. To transform the deformation back into a CAD geometry, a manual effort or approximation of the initial CAD geometry needs to be made. In the current workflow, it would mean transporting back the modified shape into the mesher (which is currently stationed outside the automatic adjoint workflow loop in Figure 2.2). Furthermore, in the case of a manual approximation, some important surface details obtained from the mesh morphing might be lost. Thus, incorporating CAD-based parametrization in the adjoint shape optimization workflow could be an option to deal with the low mesh quality within the automatic workflow in an instant manner per design iteration. On the other hand, as explained by Müller [2], other challenges appear when using this CAD-based parametrization, such as how to obtain the required derivatives of the CAD model. A variety of techniques to obtain the derivatives are proposed in [2], using CAD models such as the BRep-based models, and combined analytic shapes and Boolean operations.

- Considering the above mentioned issues, we stress that the current ANSYS Fluent adjoint optimization procedure is not mature enough for research purposes. At the moment, the ANSYS adjoint procedure is reliable only for fully laminar flow and two dimensional domain without periodic boundary condition. Thus, for a more complex case such as the one presented in Chapter 7, the ANSYS adjoint should be used after a more careful investigation. Although it is suspected that the periodic boundary condition is the main cause of the current problem of the optimizer, there is also a possibility that the flow is not fully laminar, which could lead to unsteady flow and inaccurate adjoint solutions. However, we believe that the adjoint solver is not the root cause of the problem as proven by the converged solution (Appendix A) and the correct directions of the sensitivity vectors for both objectives. Moreover, the sensitivity vectors of both objectives are not equal in magnitude nor are in exact opposite direction. A case cannot be optimized when the sensitivity vectors of both objectives are equal in magnitude and the directions are 180° difference [3]. Since there

is a possibility for a shape improvement, the root cause could be found in the step between the adjoint solver step and the mesh morphing step (see Figure 2.2). As presented in Chapter 7, the optimizer is erroneous and more investigations are needed to pinpoint the root cause of this error. For future works on shape optimization, other platforms that implement the adjoint method may offer better solutions.

Despite of its immaturity and after taking into account the overall procedure of shape optimization, ANSYS Fluent is still considered to be the most suitable platform for immediate application in industry. For example, as described by the workflow in Figure 2.2, the shape optimization procedure consists of multiple modules: the CFD solver, the adjoint solver, the optimizer, and the mesh morpher. The advantage of the current ANSYS adjoint procedure is its integrated modules that makes it applicable for a wide variety of geometries compared to in-house codes.

- In terms of application, we offer the following best-practice steps as the fastest way of optimizing a geometry. First, run the adjoint solver to obtain the sensitivity vectors and magnitudes. Second, perform the single objective optimization prior to the case of multi-objective optimization. As demonstrated in Chapter 5, the single objective optimization is of importance in order to observe the behavior of heat transfer and pressure drop of a system. As there are questions remaining about the nature of pressure drop and heat transfer for different systems, it is therefore necessary to know the dependency of these objectives on the operating conditions and the geometry. As the correlations (i.e. see Figure 5.5) are specific for a certain flow condition and heat exchanger geometry, the single-objective optimization study becomes a crucial step before performing the multi-objective optimization. This study leads to a proper weight factor selection in the subsequent step. The weighting depends on the case and sometimes it can even depend on the design iteration to find a good compromise for conflicting objectives such as the heat transfer and the pressure drop [4]. Therefore it is highly recommended to perform this study at the early stage of any optimization case. Further, it can not be generalized that the same settings of optimizing for one aerothermal system will successfully work for another system. Once the correlation of heat transfer and pressure drop dependency is obtained, combined with the sensitivity magnitudes, the approximate order of magnitude of the step sizes can be known. Third, using this magnitude information, the figure to determine the step size (e.g. Figure 7.4) can be constructed. Fourth, using information in steps 1, 2, and 3, the step sizes can be chosen. In

relation to the weight factors, it is presented in Chapter 7 that the faulty calculation of the expected change for multi-objective optimization leads to unsuccessful optimization of both objectives. It is still unclear what is the root cause of this problem, thus the utilization of ANSYS Fluent adjoint optimization procedure should be avoided when the expected values are not exactly the same as the specified step sizes for the data points in the deformed region. Once the user has confirmed that the specified step sizes result in: (1) a deformed mesh, and (2) exactly the same values of both objectives, the mesh can be morphed and then verified by rerunning the CFD solver. If the optimization procedure is confirmed to optimize both objectives, then the adjoint optimization procedure can be continued for the next design iterations.

- Although the ANSYS adjoint optimization procedure has challenges to be solved by future development, it is worth noting that the advancement achieved by the adjoint shape optimization procedure is very valuable. By performing further study on the challenges mentioned above and on the nature of heat transfer and pressure drop for the specific aerothermal system that needs to be optimized, the users can have ample possibilities of design improvement in a relatively short time. Even though some trial and error still exist in the current framework for multi-objective optimization, this method is still considered to be time-efficient in a product development process as compared to a designer's trial and error on conducting the conventionally limited parametric variation.

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Part VI

APPENDIX

APPENDIX

A.1 CONVERGENCE PLOTS AND SENSITIVITY DATA OF CHAPTER 7

Typical convergence plot for the flow and adjoint computations are given in this section. All solvers are run up to machine precision, typically with residuals lower than $1E - 10$. In relation to the failed optimization case in Chapter 7, the flow and adjoint convergence are presented in Figure A.1 and Figure A.2, respectively.

Furthermore, the sensitivity vector plots for both objectives are presented in Figure A.3. The magnitude of the vectors at the tip of the cylinders are half of the interior vectors. This is the typical problem that happens at the symmetry boundary condition, where the sensitivity magnitudes are divided by two. This information has been confirmed with the ANSYS adjoint developer.

Figure A.1: Convergence of the flow solution for cylinder array case in Chapter 7. All residuals are lower than $1E - 10$.

Figure A.2: Residual plot of the adjoint solution for cylinder array case in Chapter 7: (a) heat transfer adjoint convergence and (b) drag force adjoint convergence. All residuals are lower than $1E - 10$ except the drag force adjoint, which stabilizes around $3E - 06$ and $1E - 08$.

Figure A.3: Vector of shape sensitivity magnitude at the symmetry mesh points for cylinder array case (Chapter 7): (a) cylinder-2 and (b) cylinder-3. The magnitude at the symmetry mesh points show half of the magnitude of the interior mesh points. Vectors plotted for drag minimization.

*Social skills are not about things that can be seen by the eyes.
It is all about thoughts, emotions, mentality, sense, spiritualism,
kindness, humanity, attention, empathy, vision,
which manifest in manner and ethics.*

— Wulandari, 2018

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Finally, to all of you reading this thesis: thank you, and I wish you a life that will never be boring. Cheers!

Mahening Citra Vidya

Enschede, January 2020

CURRICULUM VITAE

MAHENING CITRA VIDYA was born in Surabaya, Indonesia, on 2 August 1990. She grew up with her parents and her only brother in her hometown until the age of 5, when she then moved to Nancy, France. At the age of 7, she returned to Surabaya, where she continued her elementary school education. She finished her junior high school, skipped one year of senior high school, and finally moved to Bandung, Indonesia, following her brother to study in Institut Teknologi Bandung (ITB).

Getting accepted in ITB in 2007, Citra spent the next five years of her life studying mechanical engineering. During this time of independence, she also got herself involved in various activities, e.g. the Mechanical Engineering Student Association, ITB Student Orchestra, and ITB Student Choir. During this time of her life, she found two passions that still burn until this day: performing music and teaching. Aside from that, she also witnessed first-hand the life of PhD students abroad at different universities and she found another burning desire in herself: studying abroad.

Having family members that mostly work in academia, it was kind of expected that her life is doomed to follow the same path. However, despite her family background, she knew that she had the longing in herself to pursue a higher degree education. Again following her brother's footsteps, she earned a scholarship, and continued her master study at the University of Twente in 2012. Ever since the first time she came to the Netherlands, she knew already that one day she would get her PhD degree. On her 29th year of existence, she finally gets it as the hardest fought birthday present she has ever given to herself.

Citra is currently living in Enschede and spending her time with her too many hobbies: playing piano, electric bass, reading, solo traveling, hiking, swimming, painting, sketching, and gardening. After finishing her PhD, she is planning to spend some time achieving her unfinished business: speaking German and running her own HPC cluster someday.

PUBLICATIONS

M.C. Vidya, N.A. Beishuizen, D. de Kleine, and T.H. van der Meer. (2019). Three-Dimensional Multi-Objective Shape Optimization of a Cylinder in a Cross-Flow Using Discrete Adjoint Method. *Proceedings of the 2nd Pacific Rim Thermal Engineering Conference, 13-17 December 2019, Maui, Hawaii*, **2** 24394.

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PROPOSITIONS

Accompanying the dissertation

MODELING AND ADJOINT OPTIMIZATION OF HEAT EXCHANGER GEOMETRIES

1. Parameters like bounding box and control points in an adjoint optimization process interfere with the final optimized geometry. – *Chapter 6*
2. The freeform deformation method in an adjoint optimization process puts a constraint on the geometry of internal structures. – *Chapter 6*
3. The best way to solve a CFD problem of transitional flow for a two-dimensional geometry with three-dimensional effects is by performing two-dimensional simulations first. – *Chapter 3*
4. The higher degree of freedom of a three-dimensional mesh above a two-dimensional mesh is prone to failure in the adjoint shape optimization procedure. – *Chapter 4-7*
5. Despite of the imperfection of numerical models, one has to aim for perfection when using them.
6. In a higher education institution, leadership by superiority is obstructing the final product of the educational system.
7. The optimum number of teachers for a course is equal to one.
8. There is an optimum number of rehearsals for a lecturer as well as for a musician to deliver the best performance.
9. To become fully culturally aware, one has to live it.
10. Too many progress meetings of a PhD increases the chance of failure.

by Mahening Citra Vidya

January 2020