A new framework for design and validation of complex heat transfer surfaces based on adjoint optimization and rapid prototyping technologies

Yukinori KAMETANI*, Yutaka FUKUDA*, Takayuki OSAWA* and Yosuke HASEGAWA*

* Institute of Industrial Science, The University of Tokyo
4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, JAPAN
E-mail: yukkam@iis.u-tokyo.ac.jp

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Abstract
In order to drastically accelerate the development processes of advanced heat exchangers, a new design framework integrating shape optimization, rapid prototyping and experimental validation is proposed. For the optimal design of heat transfer surfaces, a new adjoint-based shape optimization algorithm taking into account unsteady turbulent transport is developed. The present shape optimization algorithm is applied to two different conventional pin-fin arrays with circular cross sections so as to maximize the analogy factor, i.e., the ratio of heat transfer and pumping power for driving the fluid. The resultant optimal fin shapes are elongated in the streamwise direction and also characterized by bump-like structures formed on the upstream side of the pins. Investigation of numerical results reveals that the pressure drop of the optimal shape is significantly reduced by the suppression of vortex shedding behind the fin, whereas the heat transfer performance is maintained by the extended surface. The optimal shapes are fabricated by a resin-based additive manufacturing technique. A single-blow method allows to evaluate the heat transfer coefficient of low-thermal conductivity materials by measuring the inlet and outlet air temperature only, while the pressure loss is estimated from the pressure measurements at the upstream and downstream of the text matrix by Pitot-tubes. As a result, significant improvement of thermal hydraulic performance is experimentally confirmed for the optimal pin-fin arrays as predicted by numerical analyses.

Keywords: Shape optimization, Turbulent flow, Heat transfer, Direct numerical simulation, Single blow method

1. Introduction

Toward reducing the emission of green-house gases, the introduction of renewable energy such as wind power, solar power and geothermal heat, should be further accelerated. Despite tremendous efforts being made for achieving a sustainable society, fossil fuels still account for the major portion of energy resources in the modern society (Martinot, 2016). Heat transfer enhancement is one of key technologies to suppress the consumption of fossil fuels though improving the efficiencies of various energy devices, recovering exhaust heat from power and chemical plants, regeneration of geothermal resources, to name a few. A common strategy employed so far for enhancing heat transfer is to increase heat transfer area per unit volume by miniaturizing fluid conduits. However, such an approach is often accompanied by the increase in a pressure loss to maintain the flow, and thereby an additional irreversible loss. In addition, further miniaturization of fluid conduits is getting more and more difficult due to the constrains in manufacturing processes. Hence, there are growing needs for optimizing heat transfer surfaces for promoting convective heat transfer with a minimum pressure loss.

To date, various heat transfer surfaces have been proposed, e.g. pin-fins (Han et al., 2001), wavy-fins (Junqi, 2007), and oblique-wavy fins (Suzue et al., 2006). In these conventional designs, however, only a limited number of design parameters such as the height and pitch of fins are taken into account. Meanwhile, more sophisticated optimization techniques such as adjoint analyses (Bewley et al., 2000; Yamamoto et al., 2013) opens up a possibility of dealing with design parameters with large degrees of freedom.
Adjoint-based shape optimization was first applied to a fluid-solid interface by Pironneau (1978). Borrvall and Petersson (2003) proposed a topology optimization algorithm which can deal with the change in topology, such as making holes in solid or merging originally separated fins, by introducing a solid-density function as a design variable. Afterwards, Burger and Osher (2005) introduced a level-set function (Sussman et al., 1994) for topology optimization while keeping a solid-fluid interface sharp. More recently, the above optimization algorithm was extended to convective heat transfer problems by Alexandersen (2016). In these studies, however, a flow field is always assumed to be steady and laminar. In practical heat exchangers, however, complex heat transfer surfaces make the flow and thermal fields unsteady and turbulent even at relatively low Reynolds number, i.e., \( Re \sim O(10^2) \). Hence, the development of shape/topology optimization algorithms for turbulent flows is imperative for designing high-performance heat exchangers.

Since turbulent flows are characterized by their large degrees of freedom and unsteady nature, Reynolds-averaged Navier-Stokes (RANS) simulation with a turbulence model has been widely used for practical applications in order to reduce computational costs. Accordingly, shape optimization algorithms in the RANS framework were also developed for \( \kappa = \epsilon \) and Spalart-Allmaras models by Papoutsis-Kiachagias et al. (2015) and Yoon (2016), respectively. However, a turbulence model used in RANS often contains model constants, which are given empirically or require tuning for a specific flow configuration. Considering that the shape of a heat transfer surface and associated velocity and thermal fields around it would be drastically changed through optimization, there is no guarantee that the same model constants remain valid during the entire optimization procedures. For this reason, we develop a new strategy, in which the eddy viscosity and diffusivity are determined from direct numerical simulations (DNSs). This allows to reproduce all essential spatio-temporal scales of turbulence and calculate the eddy viscosity and diffusivity with high accuracy for each shape at the expense of the computational cost.

Even if shape/topology optimization can be achieved by the above mentioned algorithms, the resultant optimal shapes tend to be complex, so that experimental validation of their thermal hydraulic performance remains quite challenging. Recently, there have been some attempts to fabricate complex heat transfer surfaces with an additive manufacturing (AM) technology, and evaluate their heat transfer characteristics (Tasopoulos, 2005; Kirsch, 2017). Bacellar et al. (2017) validated the performance of a channel-type heat exchanger optimized through the genetic algorithm. In the above studies, the test samples were fabricated by metal-based AM techniques, and commonly suffer from non-negligible surface roughness, which causes a considerable discrepancy between numerical and experimental results. An alternative option is using polymers, which allow to fabricate complex surfaces at lower cost, and higher accuracy, though their low conductivity could be another source of errors in evaluating the overall heat transfer resistance. Arie et al. (2016) fabricated an air-water polymer exchanger by an AM technique. They showed that the thermal resistance within the polymer can be maintained sufficiently small by making a thin film. With this approach, however, only film-type geometries are allowed, so that it is difficult to exploit the full potential of shape/topology optimization with large degrees of freedom.

The single-blow method (SBM, Shumann, 1929) is a method for measuring a heat transfer coefficient at a complex surface. By instantly heating an inlet flow upstream of a heat transfer matrix, the heat transfer rate within the matrix can be estimated from the temporal response of the air temperature at the outlet. Since this method utilizes the thermal capacity of a test matrix, it can be used for low thermal conductivity materials such as polymers. Furthermore, it requires only measurements of the inlet and outlet fluid temperatures, while the temperature at a heat transfer surface is not needed. For this reason, SBM has often been applied to a heat transfer matrix with fine and complex structures. To the best of the authors’ knowledge, however, there has been no attempt to apply SBM to additively manufactured polymer heat exchangers.

In the present study, we first develop a new adjoint based shape optimization algorithm in which the eddy viscosity and diffusivity are obtained from DNS. The developed method is applied to conventional pin-fin arrays with circular cross sections in order to verify that the present optimization strategy leads to enhancement of thermal hydraulic performances. Next, the obtained optimal shapes are fabricated by a resin-based AM technique for experimental validation. We will also clarify the time-scale used for temperature measurement in SBM, in which the thermal boundary condition on a solid surface can be regarded as an isothermal condition in accordance with that imposed in the present simulation. The initial and optimal pin-fin arrays are experimentally evaluated in terms of the pressure loss and the heat transfer rate. As a result, significant enhancement of thermal hydraulic performances through the present optimization is confirmed in experiment as predicted by simulation, although there still remain quantitative disagreement between them. Finally, we close this paper with discussions on possible sources of the discrepancy.
2. Numerical procedures

2.1. Initial shape and computational domain

We consider conventional circular pin-fins arrays of two different geometries sandwiched by two parallel walls as initial shapes to be optimized. Assuming periodicities in the streamwise and spanwise directions, one periodic unit with a single pitch in the two directions is considered as illustrated in Fig. 1. We assume that air flows inside the channel with the bulk mean velocity of \( U_b = 1.5 \) m/s and the channel-half width \( \delta^* = 5 \) mm. Here, a variable with the superscript \( * \) denotes a dimensional value. The corresponding bulk Reynolds number becomes \( Re_b = U_b \delta^*/\nu^* = 500 \), where \( \nu^* \) is the kinematic viscosity of air, respectively. The streamwise, wall-normal and spanwise domain sizes of the periodic unit and the corresponding number of grid points are denoted as \((L_x^*, L_y^*, L_z^*)\) and \((N_x, N_y, N_z)\), respectively. The corresponding geometric parameters are listed in Table 1. These two configurations are chosen because they are expected to yield quite different heat transfer and pressure loss characteristics according to the empirical correlations proposed by Short et al. (2002a, 2002b). Specifically, it is expected that Case 1 yields a significantly lower pressure loss, but a slightly better heat transfer rate than Case 2. The comparison between the present results and the empirical formula will be discussed in Sec. 5.

![Initial pin-fin geometry](image_url)

Fig. 1 Initial pin-fin geometry.

| Case 1 | Case 2 |
|--------|--------|
| Diameter, \( d^* \) [mm] | 2.5 | 5.0 |
| Channel-half height, \( \delta^* \) [mm] | 5 | 5 |
| Domain size \((L_x^*, L_y^*, L_z^*)\) [mm] | (25.0, 10.0, 12.5) | (20.0, 10.0, 20.0) |
| Grid size \((N_x, N_y, N_z)\) | (240, 96, 120) | (192, 96, 192) |

2.2. Indices for thermal hydraulic performance

We evaluate the heat transfer and pressure loss characteristics with the Nusselt number, \( Nu \), and Fanning’s friction factor \( f \) multiplied with by the bulk Reynolds number \( Re_b \). Their definitions are respectively given as

\[
Nu = \frac{h^* \delta^*}{\lambda^*},
\]

\[
f = \frac{2 \Delta P^* \delta^*}{\rho^* U_b^2 L_z^*},
\]

where \( h^* \), \( \lambda^* \), \( \rho^* \) and \( \Delta P^* \) denote a heat transfer coefficient, the thermal conductivity and density of air, and a pressure drop through the channel, respectively. Here, the difference between the wall temperature and the volume average of fluid temperature \( \theta_b = \frac{1}{V} \int_V \theta dV \) is used for defining \( h^* \). \( Nu \) corresponds to a dimensionless heat transfer coefficient, where as \( f Re_b \) is a dimensionless pumping power for driving the air flow.

We also define the analogy factor as

\[
A_f = \frac{Nu}{f Re_b},
\]

which represents the ratio of heat transfer and pumping power. The purpose of the present study is to optimize the shape of a heat transfer surface so as to maximize \( A_f \) as described in Sec. 3.1.
2.3. DNS for forward simulation

In the present study, the purposes of conducting DNS for forward analysis are twofold: First, the results of DNS are used to evaluate the eddy viscosity and diffusivity, and they will be integrated to RANS equations for shape optimization. Second, the obtained heat transfer rate and pressure loss are compared with experimental results in order to validate the present simulation and the proposed optimization strategy.

2.3.1. Representation of heat transfer surface

For representing an arbitrary three-dimensional fluid-solid interface, we introduce a level-set function (Osher and Sethian, 1988), \( \phi_0(x, y, z) \), which is the signed distance function from the interface as illustrated in Fig. 2. It is defined positive and negative in the solid and fluid phases, respectively. Then, the shape indicator \( \phi(x, y, z) \) is defined based on the level-set function as

\[
\phi(x, y, z) = \begin{cases} 
0 & \left( \phi_0 \leq -\frac{\Delta}{2} \right) \\
\frac{1}{2} \left\{ \sin \left( \frac{\pi \phi_0}{\Delta} \right) + 1 \right\} & \left( |\phi_0| < \frac{\Delta}{2} \right) \\
1 & \left( \phi_0 \geq \frac{\Delta}{2} \right).
\end{cases}
\]

Accordingly, \( \phi \) becomes unity in the solid phase, whilst null in the fluid phase. The value of \( \phi \) smoothly changes from zero to unity in the interfacial region within the distance of \( \Delta/2 \) from the interface as depicted in Fig. 3. Therefore, \( \Delta \) defines the interfacial thickness, which should be sufficiently small in order to represent a sharp interface. In the present simulation, the interfacial thickness \( \Delta \) is determined so that it spans two times the diagonal grid spacing.

2.3.2. Governing equations and boundary conditions

We define the Cartesian coordinate system as \( x = (x, y, z) \) and denote the corresponding velocity components as \( u = (u, v, w)^T \), where the superscript of \( t \) indicates a transposed vector. Additionally, a static pressure and temperature are denoted by \( p \) and \( \theta \), respectively. During the optimization process, a constant mean pressure gradient is applied as a driving force and uniform heating is assumed for the thermal field. Accordingly, the governing equations for the velocity and thermal fields are the following incompressible Navier-Stokes, continuity and energy equations:

\[
\nabla \cdot \mathbf{u} = 0, \\
\frac{\partial \mathbf{u}}{\partial t} = -\nabla (\mathbf{uu}) + \nabla \left( \frac{1}{Re} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right) + \nabla p + \mathbf{\delta} - \nu \mathbf{u}, \\
\frac{\partial \theta}{\partial t} = -\nabla (\theta \mathbf{u}) + \frac{1}{Re Pr} \nabla^2 \theta + 1 - \eta \theta.
\]

\[\text{Eqn. (5)}\]

\[\text{Eqn. (6)}\]

\[\text{Eqn. (7)}\]
The governing equations are non-dimensionalized by a friction velocity based on mean pressure gradient, \( u'_c \), a friction temperature based on uniform heating source, \( \theta' \), and channel-half width \( \delta' \), respectively. The friction-based Reynolds number is set to be \( Re = u'_c \delta' / \nu' = 200 \) (Case 1), 300 (Case 2) which corresponds to an initial bulk Reynolds number of \( Re_0 = 500 \). The Prandtl number is set to \( Pr = 0.71 \). The fourth and fifth terms in the right-hand-side of Eq. (6) represent the driving force equivalent to a mean pressure gradient and an artificial body force for embedding a solid region in the Cartesian coordinate system by a volume penalization method (Goldstein et al., 1993; Schneider, 2005). Note that \( \phi \) is non-zero only in the solid phase (see, Eq. (4)), so that the damping force acts only in the solid phase in order to eliminate the fluid velocity. Similarly, an isothermal condition on the solid surface is imposed via the last term on the right-hand-side of the energy equation. A periodic boundary condition is applied to the streamwise \((x-)\) and spanwise \((z-)\) directions, while the no-slip \( u = 0 \) and iso-thermal wall \( \theta = 0 \) is applied on the two parallel walls. The grid spacings nondimensionalized by \( \delta' \) in the \( x-, y-, \) and \( z-\) directions are \((\Delta_x, \Delta_y, \Delta_z) = (2.08 \times 10^{-3}, 2.08 \times 10^{-3}, 2.08 \times 10^{-3})\) as listed in the Table 1. For spatial discretization, an energy-conservative second-order central finite difference scheme (Ham et al., 2002) is used, whereas the third-order Runge-Kutta/Crank-Nicolson scheme (Spalart et al., 1991) is applied for time integration. The calculation of pressure is decoupled from Navier-Stokes equations by the SMAC method (Amsden and Harlow, 1970).

### 2.4. Eddy viscosity and diffusivity

As mentioned in Sec. 1, the present shape optimization algorithm, which will be described in detailed in Sec. 3, is based on RANS, whereas the eddy viscosity \( \nu_r \) and diffusivity \( \alpha_r \) are determined by DNS. By introducing the Boussinesq approximation, the Reynolds shear stresses and turbulent heat flux can be expressed by \( \nu_r \) and \( \alpha_r \) as

\[
-\bar{\mathbf{uu}}' \approx \nu_r (\nabla \mathbf{u} + \nabla \mathbf{u}') = \frac{2}{3} k \mathbf{I},
\]

\[
-\bar{\mathbf{\theta u}}' \approx \alpha_r \nabla \mathbf{\theta},
\]

where \( k \) denotes the turbulent kinetic energy. The over-bar indicates time averaging, while a superscript \( ' \) denotes the deviation from the mean, i.e., a fluctuating component. Ideally, the eddy viscosity and diffusivity should be determined so as to match all the components of the Reynolds shear stress and the turbulent heat flux. In the Boussinesq approximation (8) and (9), however, it is generally not possible since the principal axes of the strain rate tensor and the Reynolds shear stress tensor (or the mean temperature gradient and turbulent heat flux) are not perfectly aligned. Therefore, in order to determine the eddy viscosity and diffusivity, we multiplied the gradient of mean velocity and thermal fields. This way, the resultant eddy viscosity and diffusivity are uniquely determined so as to reproduce the production of turbulent kinetic energy and thermal fluctuation. By taking inner product with the velocity and temperature gradient tensors, \( \nu_r \) and \( \alpha_r \) are determined as follows:

\[
\nu_r = -\frac{\bar{\mathbf{uu}}'}{\nabla \mathbf{u}} : \nabla \mathbf{u},
\]

\[
\alpha_r = -\frac{\bar{\mathbf{\theta u}}'}{\nabla \mathbf{\theta}} : \nabla \mathbf{\theta}.
\]

In the present study, both the right-hand-sides of Eqs. (10) and (11) are evaluated from the DNS results. It should be noted that the eddy viscosity and diffusivity can be negative. In order to avoid numerical instability caused by a negative diffusion coefficient, a lower limit for \( \nu_r \) and \( \alpha_r \) is set so that the effective viscosity and diffusivity do not fall below to 20% of the molecular viscosity and diffusivity, i.e.,

\[
\nu_r > \frac{0.8}{Re},
\]

\[
\alpha_r > \frac{0.8}{RePr}.
\]

### 3. Shape optimization algorithm

#### 3.1. Cost functional

We define the cost functional to be minimized as follows:

\[
\mathcal{J} = -A_f \frac{Nu}{f Re_b}.
\]

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Here, the minus sign is added, so that minimizing $J$ is equivalent to maximizing the analogy factor $A_f$. Accordingly, the current optimization problem is formulated as

$$\text{minimize} \quad J(\phi)$$

subject to

$$\mathcal{R} = 0,$$ \hspace{1cm} (15)

$$\int_{\Omega} \phi d\Omega = \text{constant}.$$ 

The second constraint is introduced to maintain the total volume of the solid phase during the optimization. $\mathcal{R}$ denotes the system-state representation of the following Reynolds-averaged governing equations.

$$\mathcal{R} = \begin{pmatrix} \nabla \cdot \bar{u} \\ \nabla (\bar{u} \cdot \bar{u}) - \nabla : \left[ v_e \left( \nabla \bar{u} + \nabla \bar{u}^T \right) \right] + \nabla \overline{p} - \delta_{11} + \eta \phi \bar{u} \\ (\alpha_c \nabla \bar{\theta}) - \nabla : \left[ \alpha_c \nabla \bar{\theta} \right] - 1 + \eta \phi \bar{\theta} \end{pmatrix} = 0,$$ \hspace{1cm} (16)

where $v_e$ and $\alpha_c$ are the sum of molecular and eddy diffusivity for momentum and heat:

$$(v_e, \alpha_c) = \left( \frac{1}{Re} + v_r, \frac{1}{Re Pr} + \alpha_t \right).$$ \hspace{1cm} (17)

Note that the above RANS equations (16) are closed by the eddy viscosity $v_r$ and diffusivity $\alpha_t$ obtained from DNS with Eqs. (10) and (11).

### 3.2. Derivation of adjoint equations

Combining the cost functional $J$ and constraints $\mathcal{R}$ with Lagrangian multipliers $\Psi = [\bar{u}, \bar{\theta}, \bar{p}]^T$, the Hamiltonian is defined as

$$\mathcal{H} = \int_{\Omega} J d\Omega - \langle \Psi, \mathcal{R} \rangle,$$ \hspace{1cm} (18)

where $\langle \cdot, \cdot \rangle$ denotes an inner product defined in the computational domain. Taking Fréchet differentiation, a change in the Hamiltonian, $\delta \mathcal{H}$ against an infinitesimal variation of shape indicator, $\delta \phi$, can be expressed as

$$\delta \mathcal{H} = \frac{D\mathcal{H}}{D\phi} \delta \phi = \frac{D\mathcal{J}}{D\phi} \delta \phi + \frac{D\mathcal{J}}{D\bar{u}} \delta \bar{u} + \frac{D\mathcal{J}}{D\bar{\theta}} \delta \bar{\theta} - \langle \Psi, \delta \mathcal{R} \rangle,$$ \hspace{1cm} (19)

where $\delta \mathcal{R}$ denotes the variational form of Reynolds-averaged governing equations $\mathcal{R}$, i.e.,

$$\delta \mathcal{R} = \frac{D\mathcal{R}}{D\phi} \delta \phi + \frac{D\mathcal{R}}{D\bar{u}} \delta \bar{u} + \frac{D\mathcal{R}}{D\bar{\theta}} \delta \bar{\theta}.$$ \hspace{1cm} (20)

Taking the Fréchet derivative of Eq. (16), $\delta \mathcal{R}$ is obtained as

$$\delta \mathcal{R} = \begin{pmatrix} \nabla \cdot \delta \bar{u} \\ \delta \bar{u} : \nabla \delta \bar{u} + \delta \bar{u} : \nabla \delta \bar{u} - \nabla : \left[ v_e \left( \nabla \delta \bar{u} + \nabla \delta \bar{u}^T \right) \right] + \nabla \delta \overline{p} + \eta \phi \delta \bar{u} + \eta \bar{u} \delta \phi \\ (\alpha_c \nabla \delta \bar{\theta}) - \nabla : \left[ \alpha_c \nabla \delta \bar{\theta} \right] - 1 + \eta \phi \delta \bar{\theta} \end{pmatrix}.$$ \hspace{1cm} (21)

Substituting Eq. (21) into Eq. (19) and factorizing with variational variables $\delta \Psi = [\delta \bar{p}, \delta \bar{u}, \delta \bar{\theta}]^T$, Eq. (19) can be rearranged as follows:

$$\delta \mathcal{H} = \langle \delta \Psi, \delta \mathcal{R} \rangle + \mathcal{B} + \mathcal{S}.$$ \hspace{1cm} (22)
where $R^i$ is given by

$$
R^i = \left\{ \begin{array}{c}
\nabla \cdot \mathbf{u}^i \\
-\mathbf{u} \cdot [\nabla \mathbf{u}^i + \nabla \mathbf{u}^i] - \nabla \cdot \left[ \nu \left( \nabla \mathbf{u}^i + \nabla \mathbf{u}^i \right) \right] + \nabla p^i + \eta \phi \mathbf{u}^i + \theta^i \nabla \theta^i - \delta_{ii} \\
\n-\mathbf{u} \cdot \nabla \theta^i - \nabla \cdot \left[ \alpha_e \nabla \theta^i \right] + \eta \phi \theta^i - 1
\end{array} \right. \quad (23)
$$

The adjoint variables $\mathbf{u}^i, p^i, \theta^i$ are obtained by solving the adjoint equations, i.e., $R^i = 0$.

The boundary term $B$ can be converted from the volume integration to the surface integration by the Gauss’ divergence theorem, so that the resultant form is given as

$$
B = \int_{\Gamma} - \left[ \nabla \mathbf{u}^i + \mathbf{u}^i \delta \mathbf{p} + (\mathbf{u}^i \cdot \delta \mathbf{u}) \mathbf{u} + (\mathbf{u}^i \cdot \mathbf{u}) \delta \mathbf{u} - \nu_e \left( \nabla \delta \mathbf{u}^i \mathbf{u}^i - (\nabla \mathbf{u}^i)^T \delta \mathbf{u} \right) + \delta \theta^i \mathbf{u} - \alpha_e \left( \theta^i \nabla \theta - \delta \theta \nabla \theta^i \right) \right] \cdot \mathbf{n} d\Gamma, \quad (24)
$$

where $\Gamma$ is the boundary of the computational domain and $\mathbf{n}$ is the unit outward normal vector on the boundary. The boundary conditions for the adjoint variables are determined so that $B = 0$. This leads to periodic boundary conditions for the streamwise and spanwise directions and the Dirichlet conditions i.e., $\mathbf{u}^i = 0$ and $\theta^i = 0$, on the two parallel walls.

When $R^i = 0$ and $B = 0$ are satisfied as mentioned above, the variation of Hamiltonian reduces to

$$
\frac{D\mathcal{H}}{D\phi} = S = \left\langle \left( \mathbf{u} \cdot \mathbf{u}^i + \delta \theta^i \right) \delta \phi \right\rangle = \left\langle \left( \mathbf{u} \cdot \mathbf{u}^i + \delta \theta^i \right) \left( \frac{d\phi}{d\phi_0} \delta \phi_0 \right) \right\rangle. \quad (25)
$$

Accordingly, minimization of $\mathcal{H}$ is achieved by iteratively updating the level set function $\phi_0$ through a steepest gradient method as follows:

$$
\phi_0^{m+1} = \phi_0^m - \beta^m \eta \left( \mathbf{u} \cdot \mathbf{u}^i + \delta \theta^i \right) \frac{d\phi}{d\phi_0}, \quad (26)
$$

where the superscript, $m$, is the number of iterations in the optimization procedure, while $\beta$ is a relaxation coefficient. In this study, $\beta$ is determined as

$$
\beta^m = \frac{0.01}{\max(|\delta \phi^m|)} \quad (27)
$$

After the update of the shape by Eq. (26), the level-set function $\phi_0$ is modified near the interfacial region and it loses the properties of a signed distance function. Hence, reinitialization of $\phi_0$ is conducted after each update of $\phi_0$ with Eq. (24). Also, in order to keep the total volume of the solid region constant, $\phi_0$ is shifted uniformly along the interface. Accordingly, the phase indicator $\phi$ is also updated based on the obtained level-set function $\phi_0$.

3.3. Summary of optimization procedures

The flowchart of the current optimization procedures is shown in Fig. 4. First, we give an initial shape, which is schematically shown in Fig. 1 with two different geometric parameters listed in Table 1. Second, we conduct DNS of velocity and thermal fields for a given structure as explained in Sec 2.3. We run computation for a sufficiently long time after the velocity and thermal fields reach fully developed state in order to obtain converged statistics. Afterwards, the eddy viscosity and diffusivity are calculated from DNS statistics based on Eqs. (10) and (11). Next, the adjoint RANS equations (21) integrated the DNS-based eddy viscosity and diffusivity are solved as described in Sec. 2.4.2. After obtaining both forward and adjoint velocity and scalar fields, the level-set function $\phi_0$ representing the shape of the solid phase is updated in accordance with Eq. (24). We iterate the above procedures until the decrease of the cost functional from a previous iteration is within 1% or the pin is detached from the parallel walls. Hereafter, we call the resultant structure the optimal shape.
4. Experimental validation

4.1. Test matrix

Both the initial and optimal pin-fin arrays are fabricated by a resin-based additive manufacturing technique based on the selective laser sintering (SLS) by Ricoh Co., Ltd. Nylon PA12 is adopted as a material due to its high fabrication precision and a large thermal capacity. The thermal properties of Nylon PA12 and air at 25°C used in the present study are summarized in Table 2. The matrix contains seven parallel channels with fins and is insulated by resin walls with the thickness of 5 cm. The schematics of matrix is illustrated in Fig. 5. Similarly, the arrangement of the original pin-arrays are shown for two cases in Fig 6. In order to suppress the pressure loss at leading edges of each channel, a super-elliptic curve is applied (Narasimha and Prasad, 1994).

Table 2  Thermal properties

| Material   | Density, $\rho$ [kg/m$^3$] | Conductivity, $\lambda$ [W/K.m] | Specific heat, $C_p$ [J/kg.K] |
|------------|-----------------------------|---------------------------------|-------------------------------|
| Nylon PA12 | $1.01 \times 10^3$          | $3.0 \times 10^{-1}$            | $1.26 \times 10^4$            |
| Air        | $6.14 \times 10^3$          | $8.66 \times 10^{-2}$           | $1.33 \times 10^3$            |

The surface of a fabricated test matrix measured by a microscope (VHX-7000, Keyence Co.) is presented in Fig. 7. It is found that the surface roughness is in the order of $0.1 \text{ mm}$. Considering that this roughness is in the order of unity in the friction length estimated from the overall pressure drop, the surface can be considered to be hydrodynamically smooth.

4.2. Single-blow method

In a single-blow method, the initially isothermal inlet flow is instantly heated up, and the resultant temperature response of the flow at the outlet is recorded to estimate the overall heat transfer rate of a test matrix (see, Fig. 9). If there were no heat exchange between the air and the test matrix, the sudden increase of temperature would be also measured.
Fig. 7  Surface of resin matrix sampled in 10 mm x 10 mm of square. Color indicates ±0.1 mm of roughness (blue to red).

Fig. 8  Experimental set-up

Fig. 9  Schematics of single blow method

at the outlet with only a time delay due to convection within a text matrix. In reality, there should exist heat exchange between the air flow and the text matrix, and therefore the resultant response at the outlet temperature becomes more gradual. In the single blow method, this outlet temperature response is used to estimate the overall heat transfer rate within the text matrix. In the following, we will introduce the experimental apparatus, and the method for estimating a heat transfer rate from the temperature response downstream.

4.2.1. Experimental apparatus

The present experimental system is composed of a wind-tunnel, a heater, and a test matrix as shown in Fig. 8. The heater located upstream of the test matrix is made of eight aluminum films. 1.5kW of electricity at maximum is applied to the heater so as to instantaneously heat up the inlet air at $t_0$ as depicted in Fig. 9. One thermocouple and nine thermocouples are installed at upstream and downstream, respectively. The sampling time is set to be two seconds, which is sufficiently long to analyze the temporal response to the inlet heating as discussed in more detail in Sec. 4.2.2. The data are sampled with the LabView software (National Instruments Co.). For each text matrix, ten measurements are performed and the average is used to estimate the heat transfer rate. As for measurement of a pressure loss, Pitot-tubes are installed at both the upstream and downstream of the matrix. Static pressure at the two locations is measured by the transducer (N239, Setra Co.) with a sampling rate of 1kHz.

4.2.2. Evaluation of heat transfer rate

In order to estimate the Nusselt number from the outlet temperature response, model curves are prepared beforehand
by using a simplified heat transfer model within a text matrix. Specifically, a conjugate heat transfer problem within the text matrix is solved by assuming a certain Nusselt number between the fluid and solid phases. The outlet temperature responses at different Nusselt numbers are numerical calculated by systematically changing the Nusselt number. Then, the Nusselt number is determined so that the measured output temperature shows best match with the model curve.

The computational domain used for the heat transfer model within a text matrix is depicted in Fig 10. The thermal field within a fluid region is treated as one dimensional, so it is only a function of the streamwise coordinate $x$. A complex heat transfer surface is not explicitly taken into account, but its effects on heat transfer are reflected in the Nusselt number $Nu$ between the fluid and solid phases. Accordingly, the governing equation for the one-dimensional temperature evolution $\theta(x)$ in the fluid region is given by

$$\frac{d\theta}{dt} = -U_b \frac{d\theta}{dx} + \frac{1}{Re_b} \frac{d^2\theta}{dx^2} + Nu \left( \theta - \theta_w \right), \quad (28)$$

The inlet temperature condition is determined from the time trace of the inlet temperature measured from the experiment, whereas the convective boundary condition is used at the outlet. In the solid phase, the following two-dimensional thermal conduction equations are considered;

$$\frac{d\theta_s}{dt} = \frac{\alpha}{Re_b} \left( \frac{\partial^2\theta_s}{\partial x^2} + \frac{\partial^2\theta_s}{\partial y^2} \right), \quad (29)$$

where $\alpha$ is the dimensionless thermal diffusion coefficient normalized by that of air. The Neumann boundary condition is applied to the outer boundaries. At the interface between air and resin, the heat flux from the air corresponding to the last term in Eq. (28) is imposed.

The heat transfer processes within the text matrix can be divided into three stages depending on the time scale after the onset of heating of the inlet air as shown in in Fig. 11. Specifically, 1) formation of a thermal boundary layer on the air side, 2) penetration of a thermal boundary layer into the solid phase, 3) temperature increase within the entire solid. During the period of 1) and the early stage of 2), the fluid-solid interface can be considered as an isothermal boundary, which is also assumed in the current DNS. The time-scale in which the wall boundary condition can be considered isothermal is determined by the thermal penetration length defined below:

$$\delta_h^* = \sqrt{\frac{\lambda^*}{\rho^* c^* t^*}}, \quad (30)$$

where the thermal conductivity $\lambda^*$, the specific heat $c^*$, and the density $\rho^*$ listed in Table 2. $t^*$ is the time after the onset of heating. In order to make the thermal penetration length sufficiently small ($\sim O(0.1)$) [mm] compared with the thickness of the solid wall, the time range of 0 $t^* < 2$[sec] is used for estimating the heat transfer rate. At $t^* = 2$[sec], the temperature of air flow increases from the room temperature by 10 degree. An example of the time evolutions of the inlet and outlet temperatures with model curves obtained by coupling Eqs. (26) and (27) at different Nusselt numbers is shown in Fig. 12. It is found that the trend of the outlet temperature evolution agrees well with those of the model curves. In this example, the Nusselt number is estimated as $Nu = 6.0$, which leads to the best match between the measurement data and the model curve. In each measurement of Nusselt number, ten independent experiments were conducted and the average of time traces of the ten measurements was used for estimating the heat transfer rate. A typical variation in the instantaneous temperature is around ±1 degree. In the present experimental condition, the above fluctuation of temperature translates to uncertainty of up to 17% in the Nusselt number.

5. Results and Discussions

5.1. Thermal hydraulic performances

The values of $fRe_b$ and $Nu$ obtained from the present simulation and experiment for the initial and optimal shapes in Cases 1 and 2 are summarized in Table 3, respectively. As for the initial shapes, we also list the reference values from the following empirical correlations proposed by Short et al. (2002a, 2002b) which are valid for $Re_d = U^*_d d/\nu^* < 1000$:

$$f = 35.1 \left( \frac{L_1}{d^*} \right)^{1.13} \left( \frac{L_2}{d^*} \right)^{-0.78} \left( \frac{2\delta^*}{d^*} \right)^{-0.55} \left( \frac{Re_b}{\delta^*} \right)^{-0.65} \left( \frac{U^*}{d^*} \right)^2, \quad (31)$$

$$Nu = 0.76Re_bPr^{1/3} \left( \frac{L_1}{d^*} \right)^{-0.16} \left( \frac{L_2}{d^*} \right)^{-0.20} \left( \frac{2\delta^*}{d^*} \right)^{-0.11} \left( \frac{Re_b}{\delta^*} \right)^{-0.67} \left( \frac{\delta^*}{d^*} \right)^2, \quad (32)$$

where $U^*_d$ denotes bulk mean velocity based on a minimum cross section.
As for $fRe_b$, it is found that the results of the present DNS and experiment, and also the empirical correlation for the initial shapes agree quite well in both Cases 1 and 2. We can also confirm good agreement between the present DNS and experiment for the optimal shapes as well. It should be noted that we applied the periodic boundary conditions in the streamwise and spanwise directions in the current DNS. Meanwhile, in the experiment, there is additional pressure loss due to the entrance and outlet regions, and also the presence of the side walls. These would be reasons why the current DNS underestimates the experimental results even for the initial shapes.

In contrast, the discrepancies in $Nu$ are generally larger. First of all, the present experimental data for $Nu$ are commonly lower than those obtained from DNS. This systematic deviation could be attributed to the difference in the thermal boundary conditions in simulation and experiment. As mentioned Sec. 4.2.2, we determine the measurement period as 2 seconds, so that the thermal penetration length into the test matrix is in the order of 0.1 mm. However, this length is not always negligibly small compared with the local minimum thickness of a fin, especially for the optimal shapes, which exhibit more complex and thinner structures as shown in Sec. 5.2. As a result, it is expected that the temperature of the heat transfer surface is not exactly in an isothermal condition, but gradually heated up during the measurement period. This reduces the actual temperature difference between the fluid and the heat transfer surface, and thereby the resultant Nusselt number in the experiment. We also note that the effects of the entrance region and
Table 3  Summary of thermal hydraulic performances obtained from the present DNS and experiment (EXP) for initial (init.) and optimal (opt.) shapes in Cases 1 and 2. The empirical correlations for the initial shapes by Short et al. (2002a,"1) and Short et al. (2002b,"2) are also listed for comparison. The parenthesized values indicate the ratio of the changes from initial to optimal shapes.

| Case   | Re_b  | Nu   | A_f  | Re_b  | Nu   | A_f  | Re_b  | Nu   | A_f  |
|--------|-------|------|------|-------|------|------|-------|------|------|
|        | DNS   | EXP  | Ref."1| DNS   | EXP  | Ref."2| DNS   | EXP  | Ref."3"|
| 1 (init.) | 121.2 | 142.8 | 86.0 | 13.9 | 8.0 | 13.8 | 0.115 | 0.056 | 0.160 |
| 1 (opt.) | 67.3 (−44%) | 70.1 (−51%) | – | 13.5 (−3%) | 6.0 (−25%) | – | 0.201 (+75%) | 0.086 (+54%) | – |
| 2 (init.) | 190.0 | 226.5 | 171.4 | 15.5 | 10.0 | 7.9 | 0.082 | 0.044 | 0.046 |
| 2 (opt.) | 158.1 (−17%) | 163.4 (−28%) | – | 13.8 (−12%) | 10.0 (±0%) | – | 0.087 (+6%) | 0.061 (+39%) | – |

Fig. 13 2Nu versus fRe_b for initial and optimal shapes. Solid and open symbols denote initial and optimal shapes, respectively. Grey lines are iso-contours of Nu/(fRe_b) spacing at 0.01.

the spanwise walls are not taken into account in the present simulation due to the periodic boundary conditions in the streamwise and spanwise directions. Even though such quantitative differences exist, however, the trend that the reduction of Nu is generally weaker than that of fRe_b in the simulation is captured in the present experiment. For the initial shape in Case 1, the correlation Eq. (32) predicts well the present DNS result. On the other hand, the correlation Eq. (32) provides significantly lower Nu that that obtained in the present DNS for the initial shape of Case 2. This may be explained by the present Reynolds number, which suggests that the current flow is in the transitional regime. It is possible that the correlation Eq. (32) fail to predict laminar-turbulence transition, and associated heat transfer enhancement in Case 2.

Although Nu is slightly reduced after optimization, fRe_b is more significantly suppressed, so that the analogy factor A_f is enhanced for the optimal shapes in both Cases 1 and 2 as shown in Table 3. The increase of A_f is more prominent in Case 1. Specifically, A_f is increased by around 75% (54%) for Case 1 and 6% (39%) for Case 2 in DNS (experiment). The thermal hydraulic performances of the present initial and optimal shapes are compared in the 2Nu – fRe_b map shown in Fig. 13. The grey lines are isolines of A_f and the diagonal solid black line corresponds to A_f = 1. The purpose of the present optimization is to move the performance of an initial shape toward the up-left direction in the figure. It is confirmed that similar trends of performance enhancement in Cases 1 and 2 by the present optimization strategy are observed in both present simulation and experiment.

5.2. Optimal shapes and mechanisms of performance enhancement

The optimal structures obtained from Cases 1 and 2 are depicted by white surface in Fig. 14. The corresponding initial shapes are also drawn by transparent purple surfaces in order to highlight the differences between the initial and optimal shapes. It is found that the optimal shape in Case 1 is extended toward the upstream direction, and there are two protrusions, which are symmetric in the wall-normal direction. On the other hand, the optimal shape in Case 2 possesses a pair of fins in the spanwise direction. Also, there are totally four protrusions in the wall-normal directions. Hence, although the overall trends such as generation of bump-like structures on the upstream side of the fin, and elongation of the initial fin in the streamwise direction, are similar in Cases 1 and 2, the final optimal structures are different. This is because the present optimization strategy is based on a gradient method, so that the results are generally dependent of the initial condition.
In order to discuss the mechanisms of performance enhancement in the optimal structures, the mean streamwise velocity at the channel center is depicted in Fig. 15. It is found that, both in Cases 1 and 2, the streamwise velocity is increased especially at downstream of the optimized fins. Furthermore, the spatial distributions of the Reynolds shear stress, \( \overline{w'u'} \), in both Case 1 and Case 2 obtained by the DNS are depicted in Fig. 16. It is confirmed that \( \overline{w'u'} \) is reduced in the optimal structure. This fact indicates that suppression of the Kármán vortex shedding leads to the reduction of a pressure loss. On the other hand, Fig. 17 indicates that the local heat flux is enhanced around the bumps on the upstream side of the optimized pins in Case 2. This contributes to maintain the heat exchange between the air and the fin even though significant reduction of a pressure loss is achieved in the optimal shape. Similar trend can be found in Case 1.

6. Conclusions

We proposed a new adjoint-based shape optimization algorithm for turbulent convective heat transfer. The unique feature of the present algorithm is to use DNS for evaluating the eddy viscosity and diffusivity, so that the present scheme does not rely on any turbulence model. The proposed optimization strategy was applied to two different geometries of pin-fin arrays, and significant enhancement of thermal hydraulic performance was confirmed.

Next, we fabricated the initial and optimal heat transfer surfaces with a resin-based additive manufacturing technique in order to validate their performances. As a results, significant increase of the analogy factor by 54% and 39% were experimentally obtained for initially thin (Case1) and thick (Case2) pin fin arrays, respectively. Flow visualization reveals that the optimal shapes suppress Kármán vortex shedding behind a pin-fin, and this contributes to the reduction of the pressure loss. Meanwhile, the heat transfer is enhanced on the upstream side of the fin where the bump-like structures forms in the optimal structure. Although similar performance enhancement in \( A_f \) was obtain in both simulation and simulation, there still exists quantitative discrepancy between them, especially for the Nusselt number. This should be mostly attributed to the fact that the thermal penetration depth is not small enough in comparison to the length-scale of
the solid phase, so that the thermal boundary condition at the fluid-solid interface is no longer regarded as an isothermal condition assumed in the present simulation. This discrepancy could be mitigated by introducing a new material with larger thermal capacity and lower thermal conduction, or taking into account conjugate heat transfer in DNS. They remain to be addressed in future work.

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