

Optimal air distribution design in enclosed spaces using an adjoint method

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This investigation studied an adjoint method to achieve the optimal design of ventilation in an enclosed environment and validated it with two, two-dimensional cases. A part of the flow field and/or temperature field was defined as the design objective, and the thermo-fluid boundary conditions were determined as the design variables. By using the adjoint method together with a steepest descent method that was implemented in OpenFOAM, this investigation found the optimal air supply parameters. With the determined air supply parameters, this study used CFD to calculate the flow and/or temperature fields, which are in a good agreement with the design objective. However, as the adjoint method could only find the local optima, the calculations with different initial inlet air conditions may lead to multiple optimal solutions. This is common with the gradient-based method.

Keywords: inverse design, optimal control, ventilation, inlet boundary conditions, adjoint method

1. Introduction

Ventilation is one of the most important factors in maintaining an acceptable indoor environment in enclosed spaces such as buildings and transportation vehicles. Ventilation can control the air temperature, relative humidity, air speed, and chemical species concentrations in the air of enclosed spaces. There are many standards [1] for formulating the requirements of an indoor environment, and ventilation design should be optimized for creating and maintaining an environment to satisfy the requirements.

Traditionally, researchers and engineers have applied a "trial-and-error" process in designing ventilation, which means predicting and evaluating ventilation performance with different design variables to find the scenario that best agrees with the design objective. According to Chen [2], researchers and engineers have typically predicted or evaluated ventilation performance by analytical and empirical models, experimental measurements, and computer simulations. With the development of computer technology, Computational Fluid Dynamics (CFD) simulations have recently been the most popular method of predicting ventilation performance. A CFD simulation can provide field distributions of air velocity, air temperature, species, etc. With a validated turbulence model, a CFD simulation would be more accurate and informative than analytical models, empirical models, multizone models, and zonal models and much faster than experimental measurements. However, because this "trial-and-error" process requires CFD simulations for a large number of scenarios, it would take days or months to obtain an optimal design for a ventilated space. At the same time, a "trial-and-error" process with the other methods may be inaccurate, non-informative, expensive, and/or time-consuming. Most importantly, because of the subtlety and complexity of fluid flow, it is unlikely that repeated trials in an interactive analysis and design procedure would lead to a truly optimal design. By eliminating the notion of this "trial-and-error" process, the optimization approach could achieve this design goal.

The optimization approach has been widely applied in identifying a groundwater pollution source, in a linear optimization method [3], maximum likelihood method [4], and nonlinear

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50 optimization method [5]. Generally, there are two main categories of optimization approach:
 51 the gradient-based method and the gradient-free method. The gradient-free method such as
 52 Genetic Algorithms (GA) [6] uses a population of solutions and is useful when the function
 53 optimized is not differentiable or when it is expected that many local optima exist. But it still
 54 requires too many CFD simulations. The gradient-based method such as adjoint method
 55 computes the derivative of the design objective with respect to the design variables to
 56 determine the search direction. Therefore, this method normally could only find the local
 57 optima, but it requires less computing load than the GA. An approach involving the solution
 58 of an adjoint system of equations has recently attracted substantial interest from
 59 mathematicians and computational scientists. Systematic mathematical and numerical analysis
 60 of optimal control problems of different types are available, such as Dirichlet, Neumann, and
 61 distributed controls, as well as finite-dimensional controls for the steady state Navier-Stokes
 62 system [6,7,8]. For the time-dependent Navier-Stokes system, Cuverlier [9] conducted a
 63 mathematical treatment of the optimal boundary for heat flux control with free convection.
 64 The existence of optimal solutions was proven, and necessary conditions were derived for
 65 characterizing optimal controls and states. Jameson [10,11] developed an adjoint approach for
 66 potential flow. He used Euler equations and Navier–Stokes equations to find the geometry
 67 that minimizes some objective function subject to a set of constraints. Gunzburger [12] built
 68 up adjoint equations and their solving method for suppression of instabilities in boundary
 69 layer flows using injection or suction control and a stress-matching problem [13]. The
 70 optimization approach solved by the adjoint method shows great potential (i.e., fast and
 71 optimal). Multiple parameters can be combined in the optimal design of ventilation in an
 72 enclosed environment.

73 Because of the successes in previous studies, this investigation established an adjoint
 74 method for the optimal design of indoor airflow with thermo-fluid boundary conditions as the
 75 causal aspect and flow and/or temperature fields as the design objective. By implementing this
 76 method in the CFD solver OpenFOAM (Open Field Operation And Manipulation) [14], this
 77 study determined the air-supply parameters in two, two-dimensional ventilated spaces.
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79 **2. Method**

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 81 To apply the optimization approach, this study first transformed the design problem into a
 82 control problem. Then an adjoint system could be established and implemented in
 83 OpenFOAM.
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85 **2.1. Design problem as control problem**

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 87 In ventilation design, the thermo-fluid boundary conditions are design variables, and flow
 88 and/or temperature fields are the design objective. Thus, the control problem consists of the
 89 following components:
 90

- 91 • State variables: velocity V , pressure p , temperature T ;
- 92 • Design variables: inlet air velocity V_{inlet} and inlet air temperature T_{inlet} ;
- 93 • State equations: Navier-stokes equations denoted by $S = (S_1, S_2, S_3, S_4, S_5)$ and:

$$94 \quad S_1 = -\nabla \cdot V = 0 \quad (1)$$

$$(S_2, S_3, S_4)^T = (V \cdot \nabla)V + \nabla p - \nabla \cdot (2\nu D(V)) - \gamma \bar{g}(T - T_{op}) = 0 \quad (2)$$

$$S_5 = \nabla \cdot (VT) - \nabla \cdot (\kappa \nabla T) = 0 \quad (3)$$

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- Objective function:

$$J(V_{inlet}, T_{inlet}) = \alpha \int_{\theta_1} (V - V_0)^2 d\theta_1 + \beta \int_{\theta_2} (T - T_0)^2 d\theta_2 \quad (4)$$

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In the state equations, $S_1, S_2, S_3, S_4,$ and S_5 are vector components of S ; ν is the effective viscosity; $D(V) = (\nabla V + (\nabla V)^T) / 2$ is the rate of strain tensor; κ is the effective conductivity; $T_{op} = 291.5$ K that is the operating temperature; $\gamma = 0.00343$ that is the thermal expansion coefficient of the air; and $\vec{g} = (0, 0, 9.81)$ m/s² that is the gravity vector. In the objective function, velocity distribution V_0 on domain θ_1 and temperature distribution T_0 on domain θ_2 are the design objective, and V and T are calculated from the state function. α and β are chosen to adjust the relative importance of the two integrals in equation (4). The Boussinesq approximation is applied to simulate the thermal effect, while air density is assumed constant, which has been a common approach for room airflow simulations. Then, the optimization approach is to minimize objective function $J(V_{inlet}, T_{inlet})$ subject to the state equations.

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110 2.2. Adjoint equations

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112 With the introduction of a Lagrangian function L , the constrained control problem can be
113 transformed into an unconstrained control problem. An augmented objective could be:

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$$L = J + \int_{\Omega} (p_a, V_a, T_a) S d\Omega \quad (5)$$

115

116 where Ω stands for the flow domain, V_a the adjoint velocity, p_a the adjoint pressure, and T_a the
117 adjoint temperature. These parameters are Lagrangian multipliers. The integrand on the right
118 hand side of Equation (5) is the dot product of vector (p_a, V_a, T_a) and vector S . Then the total
119 variation of L is:

120

$$\delta L = \delta_{V_{inlet}} L + \delta_{T_{inlet}} L + \delta_V L + \delta_p L + \delta_T L \quad (6)$$

121

122 which includes the contributions from changes in V_{inlet} and T_{inlet} and the corresponding
123 changes in state variables $V, p,$ and T . The state equations should be calculated once for each
124 variable in order to satisfy $S = 0$. To find the relationship between the variations of V_{inlet} and
125 T_{inlet} and the δL , the adjoint velocity V_a , the adjoint pressure p_a , and the adjoint temperature T_a
126 are chosen to satisfy:

127

$$\delta_V L + \delta_p L + \delta_T L = 0 \quad (7)$$

128

129 Based on equation (7), this study has developed the adjoint equations. The reader can refer
130 to Othmer [15] for the detailed derivation procedure. In the current paper, only the adjoint
131 equations in final form are presented, as follows:

132

$$-\nabla \cdot V_a = 0 \quad (8)$$

$$-\nabla V_a \cdot V - (V \cdot \nabla) V_a - \nabla \cdot (2\nu D(V_a)) + \nabla p_a - T \nabla T_a + 2\alpha(V - V_0) = 0 \text{ for domain } \theta_1 \quad (9)$$

$$-\nabla V_a \cdot V - (V \cdot \nabla) V_a - \nabla \cdot (2\nu D(V_a)) + \nabla p_a - T \nabla T_a = 0 \text{ for domain } \Omega \setminus \theta_1 \quad (10)$$

$$-V \cdot \nabla T_a - \nabla \cdot (\kappa \nabla T_a) + 2\beta(T - T_0) = 0 \text{ for domain } \theta_2 \quad (11)$$

$$-V \cdot \nabla T_a - \nabla \cdot (\kappa \nabla T_a) = 0 \text{ for domain } \Omega \setminus \theta_2 \quad (12)$$

133

134 The term $T \nabla T_a$ in Equation (9) and (10) cancels when $\beta = 0$ in the objective function. To
 135 insure the convergence of the adjoint momentum equation, this study neglected this term in
 136 the calculations.

137 At the same time, this investigation has developed the corresponding adjoint boundary
 138 conditions. At the inlet and wall, the adjoint velocity boundary condition is $V_a|_{inlet, wall} = 0$ and
 139 the adjoint pressure boundary condition is zero gradient. At the outlet, the adjoint velocity and
 140 pressure boundary conditions are:

141

$$V_{at} V_n + \nu(\vec{n} \cdot \nabla) V_{at} = 0 \quad (13)$$

$$(\vec{n} \cdot \nabla) V_{an} = -\nabla_t \cdot V_{at} \quad (14)$$

$$p_a = V_a \cdot V + V_{an} V_n + \nu(\vec{n} \cdot \nabla) V_{an} \quad (15)$$

142

143 The subscripts t and n refer to the tangential and normal components, respectively. At the
 144 wall, the adjoint temperature boundary condition of zero gradient is applied. At the inlet and
 145 outlet, this study calculated the temperature as:

146

$$T_a V_n + \kappa(\vec{n} \cdot \nabla) T_a = 0 \quad (16)$$

147

148 According to Equations (6) and (7), the variation of L is calculated as

149

$$\delta L = \delta_{V_{inlet}} L + \delta_{T_{inlet}} L = \delta_{V_{inlet}} J + \delta_{T_{inlet}} J + \int_{\Omega} (p_a, V_a, T_a) \delta_{V_{inlet}} S d\Omega + \int_{\Omega} (p_a, V_a, T_a) \delta_{T_{inlet}} S d\Omega \quad (17)$$

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151 Thus, the sensitivity of the augmented objective becomes:

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$$\frac{\delta L}{\delta V_{inlet}} = \int_{\Omega} (p_a, V_a, T_a) \frac{\partial S}{\partial V_{inlet}} d\Omega \quad (18)$$

$$\frac{\delta L}{\delta T_{inlet}} = \int_{\Omega} (p_a, V_a, T_a) \frac{\partial S}{\partial T_{inlet}} d\Omega \quad (19)$$

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154 We set

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$$\delta V_{inlet} = -\lambda_1 \left[\int_{\Omega} (p_a, V_a, T_a) \frac{\partial S}{\partial V_{inlet}} d\Omega \right]^T \quad (20)$$

$$\delta T_{inlet} = -\lambda_2 \left[\int_{\Omega} (p_a, V_a, T_a) \frac{\partial S}{\partial T_{inlet}} d\Omega \right]^T \quad (21)$$

156

157 where λ_1 and λ_2 are positive constants. The integrands in Equation (18) and (20) are product
 158 of a vector and a matrix, and those in Equation (17), (19), and (21) are product of two vectors.
 159 The variation of L is always negative, and the value of L always decreases until an optimum
 160 condition is achieved. Therefore, using the simple steepest descent algorithm, the variation of
 161 V_{inlet} and T_{inlet} at the boundary face cell can be written approximately as:

162

$$\delta V_{inlet}^i = -\lambda_1 [V_{inlet}^i \cdot V_{a(inlet)}^i - (\nabla T_{inlet})^i T_{a(inlet)}] \quad (22)$$

$$\delta T_{inlet} = -\lambda_2 (-\gamma \vec{g} \cdot V_{a(inlet)} + \vec{n} \cdot V_{inlet} T_{a(inlet)}) \quad (23)$$

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where $V_{a(inlet)}$ and $T_{a(inlet)}$ are the calculated adjoint velocity and temperature, respectively, at the cell adjacent to the corresponding boundary face cell. The superscript i denotes a vector component.

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2.3. Numerical method

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Figure 1 shows that the calculation begins with an initial guessed inlet boundary condition of air velocity and temperature. With the initial boundary condition, our method first solves the state equations with N_1 iterations. Next, the method evaluates the objective function J . If J is smaller than a small constant ε set by the designer, the calculation stops, or this method initializes and calculates the adjoint equations with N_2 iterations. Based on the results of the state equations and adjoint equations, one can compute the variation of the inlet air velocity and temperature and obtain a new inlet air conditions. This creates a design cycle. After the first design cycle, the convergence criterion would be $|J - J_{old}| < \zeta$ instead, where J_{old} is the computed objective function in the prior design cycle and ζ is also a small constant that set by the designer. The new boundary conditions are used to calculate the state equations again until the convergence criterion is satisfied.

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N_1 and N_2 are the number of iterations for solving the state equations and adjoint equations, respectively, until they converge in each design cycle. However, N_1 and N_2 can also equal to one, where the updating of boundary conditions use partially converged state and adjoint solutions to calculate the sensitivities that is an all-at-once or one-shot method.

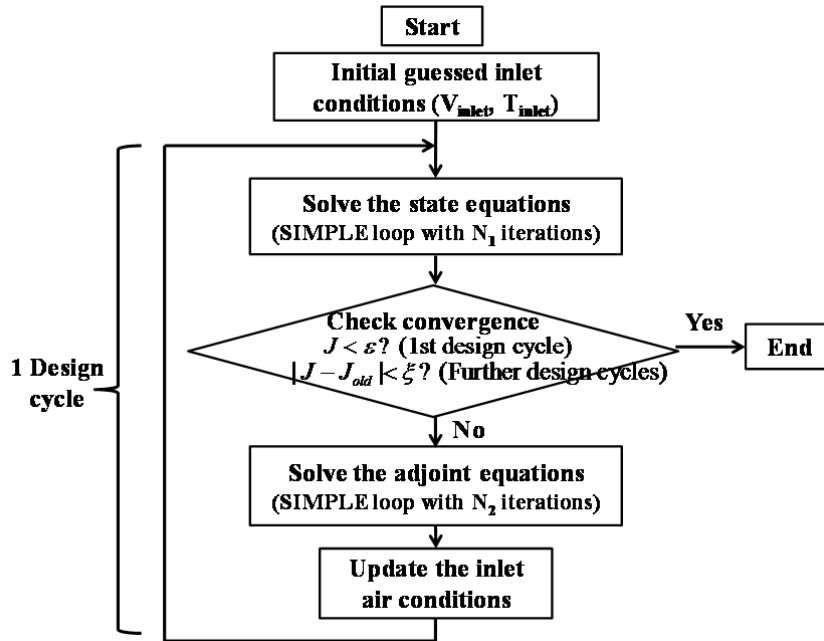
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The solver uses a Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) [16] algorithm to couple the velocity/adjoint velocity and pressure/adjoint pressure in solving the state/adjoint equations.



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Figure 1. Solution flow chart for the adjoint method

192 This investigation applied the standard k-ε model [17] to simulate turbulence in the state
 193 equations. To decrease the calculation load, this study assumed the turbulence to be “frozen”
 194 [15,18], and the turbulent viscosity in the state equations was re-used for the adjoint diffusion
 195 term. For the convection terms, this study adopted the standard finite volume discretisation of
 196 Gaussian integration with the first-order upwind-differencing-interpolation (Gauss Upwind)
 197 scheme [19]. The diffusion terms adopted the standard finite volume discretisation of
 198 Gaussian integration with the central-differencing-interpolation (Gauss Linear) scheme. The
 199 adjoint equations applied the Gauss Linear scheme for the gradient term. Neither the Gauss
 200 upwind scheme nor the Gauss liner scheme is the most accurate, but these two schemes can
 201 make the calculation stable. This investigation solved the state and adjoint continuity
 202 equations by the generalized Geometric-Algebraic Multi-Grid (GAMG) [20] solver. GAMG is
 203 faster than standard methods when the increase in speed by solving first on coarser meshes
 204 outweighs the additional costs of mesh refinement and mapping of field data. The adjoint
 205 method was implemented in OpenFOAM, which is a CFD toolbox and can be used to
 206 simulate a broad range of physical problems.
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208 3. Results

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210 This study has validated the adjoint method by applying it to two, two-dimensional
 211 ventilation cases, one with isothermal flow and the other with non-isothermal flow.
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213 3.1. Isothermal case

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215 This case was from Nielsen [21], who provided detailed experimental data. As the inlet air
 216 temperature and the wall temperature were identical and no heat sources in the cavity, it is an
 217 isothermal case as the temperature is uniform throughout the cavity. Therefore, this study did
 218 not consider the energy equation and adjoint adjoint equation in this case. Figure 2 shows
 219 the geometry of this case, where L/H=3.0, h/H=0.056, and t/H=0.16, and where H=3.0 m. It
 220 also shows the mesh used in the calculations. The inlet velocity was $V_x=0.455$ m/s and $V_y=0$
 221 with a turbulence intensity(TI) of 4% that is computed by [22]:
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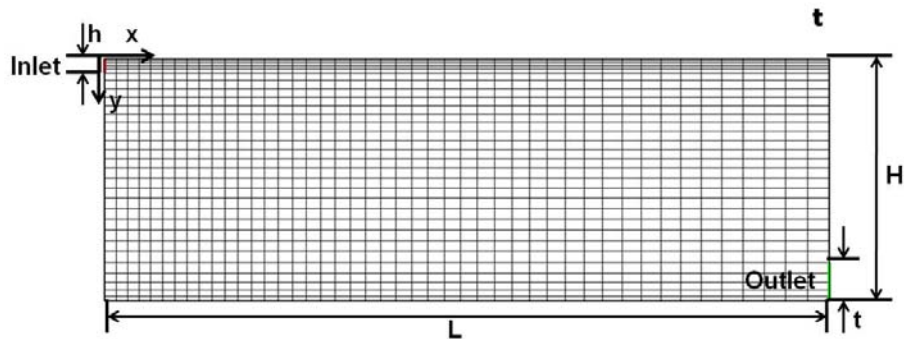
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$$TI = V' / \bar{V} = \sqrt{\frac{1}{3}(V_x'^2 + V_y'^2 + V_z'^2)} / \bar{V} \quad (24)$$

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224 where the prime denotes the turbulent fluctuation and the bar denotes the averaged value.
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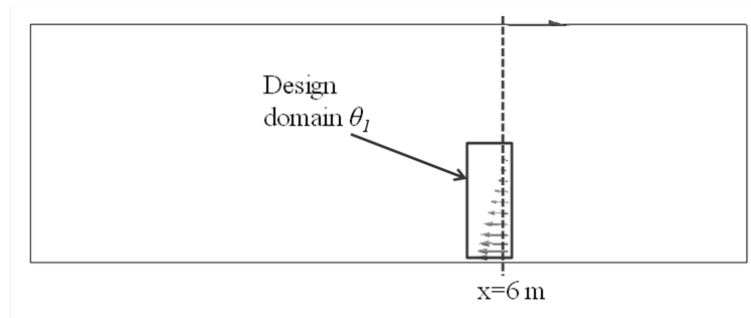
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Figure 2. Sketch and mesh of the two-dimensional isothermal case.

229 This study first conducted a forward CFD simulation with the standard k-ε model by
 230 assigning the inlet air velocity as $V_x=0.455$ m/s and $V_y=0$ corresponding to Reynolds number
 231 (Re):

$$232 \quad \text{Re} = \frac{hV_x}{\nu} = 5000 \quad (25)$$

233 where kinematic viscosity ν for air is 15.3×10^{-6} m²/s in this case. The forward CFD
 234 simulation was performed to obtain a flow field in the room, and a section of it can be used as
 235 the design objective. Figure 3 shows the computed air velocity profile (V_0 in Equation (4)) at
 236 the lower section of line $x=6$ m (design domain θ_1) that was selected as the design objective.
 237 So in the objective function (Equation (4)), this study set $\alpha = 1$ and $\beta = 0$. Next, this study
 238 aimed to find the optimal inlet air velocity based on this design objective. As the design
 239 objective was produced by the assigned inlet air velocity of $V_x = 0.455$ m/s and $V_y = 0$, this
 240 value is the most optimal and the optimized inlet air velocity may be the same as this value.
 241 However, the solution may lead to other values as long as the objective is reached.
 242



244 Figure 3. Design objective for the two-dimensional isothermal case

245 Because the isothermal case was simple, the adjoint method could lead to a converged
 246 solution in a limited number of iterations. For simplicity, this study used $N_1=N_2=1$ (see Figure
 247 1) in the calculation. This investigation used four different inlet air velocities as the initial
 248 inlet conditions, which were different from the true value of $V_x = 0.455$ m/s and $V_y = 0.0$ m/s:
 249

- 250 (1) $V_x = 1.0$ m/s and $V_y = 0.0$ m/s
- 251 (2) $V_x = 1.0$ m/s and $V_y = 0.1$ m/s
- 252 (3) $V_x = 1.0$ m/s and $V_y = -0.1$ m/s
- 253 (4) $V_x = 1.0$ m/s and $V_y = 0.3$ m/s

254 With the initial boundary conditions, the flow and adjoint equations were calculated for
 255 2000 design cycles with $N_1=N_2=1$. Figures 4 and 5 show that the first three initial conditions
 256 gradually changed to the true result of $V_x = 0.455$ m/s and $V_y = 0.0$ m/s. The error for V_x was
 257 as small as 0.25-1.8%. The error for V_x was as small as 0.25-1.8%, and the calculated V_y was
 258 exactly 0.0 m/s. Unexpectedly, the calculation with an initial velocity of $V_x = 1.0$ m/s and V_y
 259 = 0.3 m/s led to a final velocity of $V_x = 0.132$ m/s and $V_y = 2.578$ m/s. Figure 6 further shows
 260 that all the calculations could lead to a small value of the objective function. Figures 4-6
 261 illustrate that the calculations at the beginning were unstable. This was caused by the partially
 262 converged flow field and adjoint equations as $N_1=N_2=1$. The calculation was also unstable
 263 when the cycle number equalled 500, and it was difficult to identify the exact cause.
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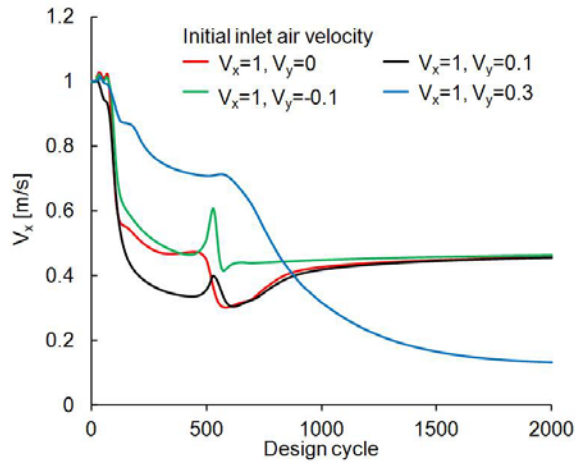


Figure 4. Change in V_x with the design cycle

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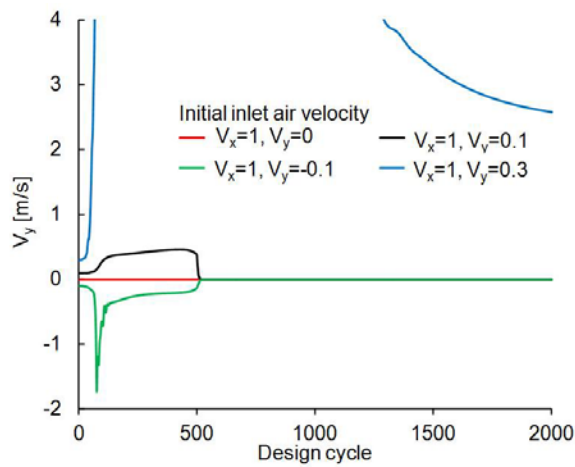


Figure 5. Change in V_y with the design cycle

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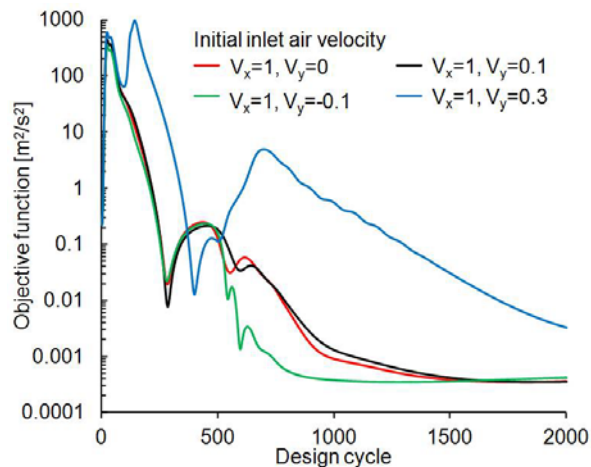
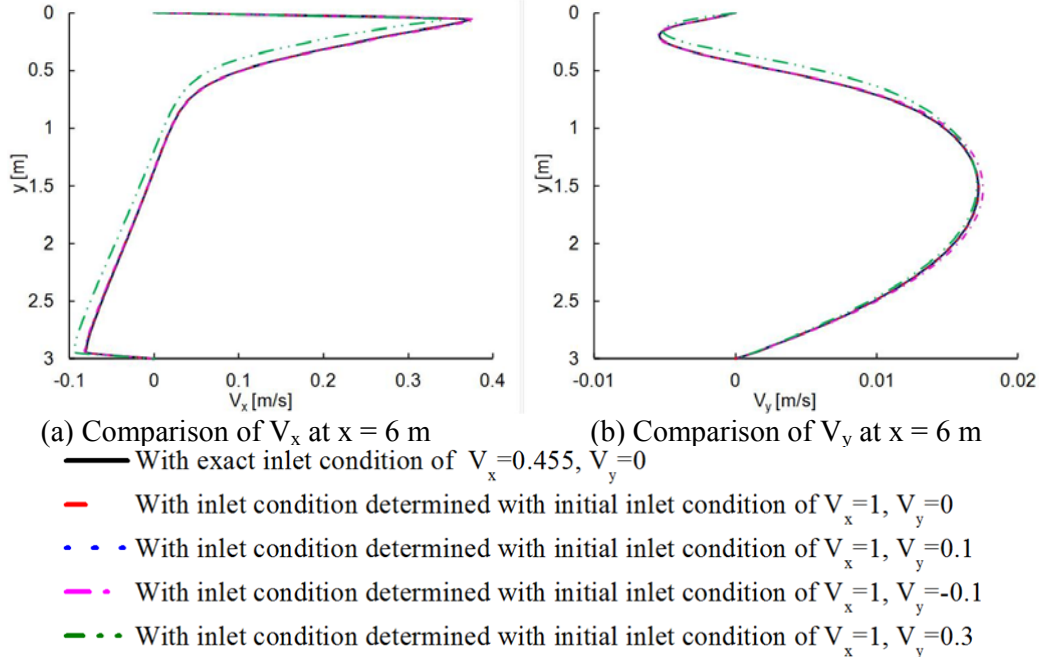


Figure 6. Change in the objective function with the design cycle

277 This study then conducted forward CFD simulations with the inlet air velocities
278 determined by the adjoint method. Figure 7 compares the computed velocity profiles at $x = 6$
279 m with the profile computed by the exact inlet air velocity of $V_x=0.455$ m/s and $V_y=0$ m/s.
280 Only the calculation with an inlet velocity of $V_x=0.132$ m/s and $V_y = 2.578$ m/s displayed a

281 minor difference. Therefore, this adjoint method can find the optimal inlet air velocity with a
 282 small value of the objective function. In other words, the adjoint method can inversely find the
 283 desired inlet air velocity by setting the velocity profile in the lower part of $x = 6$ m as the
 284 design objective. However, the results show that in order to achieve the design objective, the
 285 solution may not be unique.
 286



289
 290 Figure 7. Comparison of the design objective (velocity profiles) determined by the adjoint
 291 method and that determined by the specified inlet condition of $V_x = 0.455$ m/s, $V_y = 0$ m/s at x
 292 $= 6$ m.
 293

294 3.2. Non-isothermal case

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 296 This investigation also applied the adjoint method to a two-dimensional, non-isothermal
 297 case as shown in Figure 8. The dimensions of the flow domain were 1.04 m \times 1.04 m, the
 298 inlet height was $h = 18$ mm, and the outlet height was $t = 24$ mm. The inlet air velocity was V_x
 299 $= 0.57$ m/s, $V_y = 0.0$ m/s, and the inlet air temperature (T_{inlet}) was 15°C . The temperature of
 300 the walls (T_{wall}) was 15°C , and that of the floor (T_{fl}) was 35°C . Figure 8 also shows the
 301 resolution of the mesh used in the numerical simulation. Blay et al. [23] conducted
 302 experimental measurements of the airflow and temperature distributions for this case.
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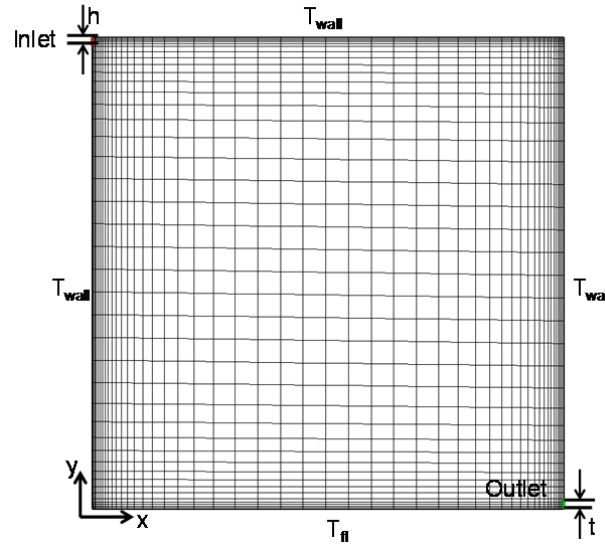


Figure 8. Sketch and mesh of the two-dimensional, non-isothermal case.

Again, this study conducted a CFD simulation with inlet air velocity $V_x = 0.57$ m/s and $V_y = 0.0$ and inlet air temperature of 15°C to generate a design objective. The design objective selected for this case was the air velocity profile (V_θ in Equation (4)) and/or air temperature profile (T_θ in Equation (4)) at mid-cavity (design domain $\theta_1 = \theta_2$) as shown by the red line in Figure 9:

- Scenario 1: Air velocity profile
- Scenario 2: Air temperature profile
- Scenario 3: Air velocity and temperature profiles

The design variables were the inlet air temperature and velocity. For Scenario 3, to adjust the importance of the velocity error and temperature error in the objective function, this study normalized the velocity error by the exact inlet air velocity $V_x = 0.57$ m/s and the temperature error by $(T_{fl} - T_{inlet})$. So we have:

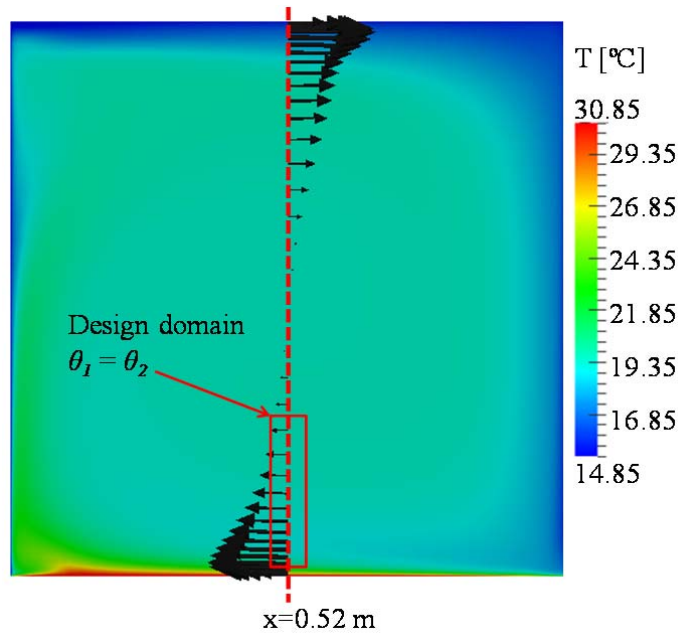
$$\alpha = \frac{1}{V_x^2}; \beta = \frac{1}{(T_{fl} - T_{inlet})^2} \quad (26)$$

Table 1 summarized the initial inlet air conditions for each scenario:

Table 1. Initial inlet air conditions for each scenario.

	Case	Initial inlet air temperature ($^\circ\text{C}$)	Initial inlet air velocity (m/s)
Scenario 1	1a	$T = 6.85$	$V_x = 1.0,$ $V_y = 0.5$
	1b	$T = 21.85$	
Scenario 2	2a	$T = 6.85$	
	2b	$T = 21.85$	
Scenario 3	3a	$T = 6.85$	
	3b	$T = 21.85$	

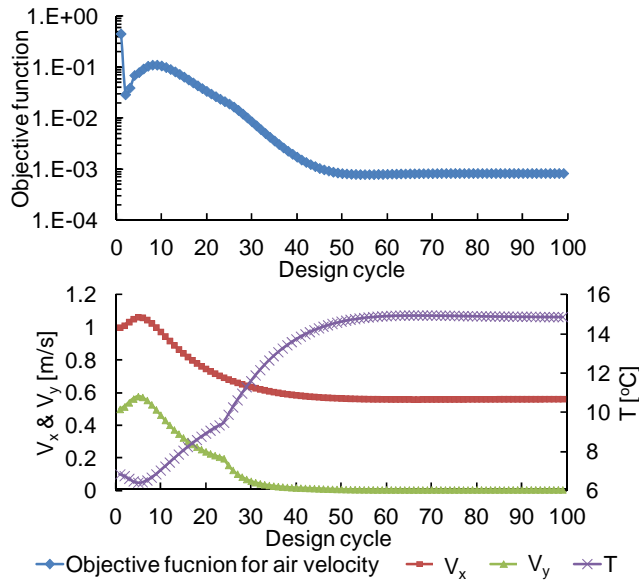
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328 Figure 9. Design objective for the two-dimensional, non-isothermal case: velocity and/or
329 temperature profiles at mid-cavity as shown by the red line.
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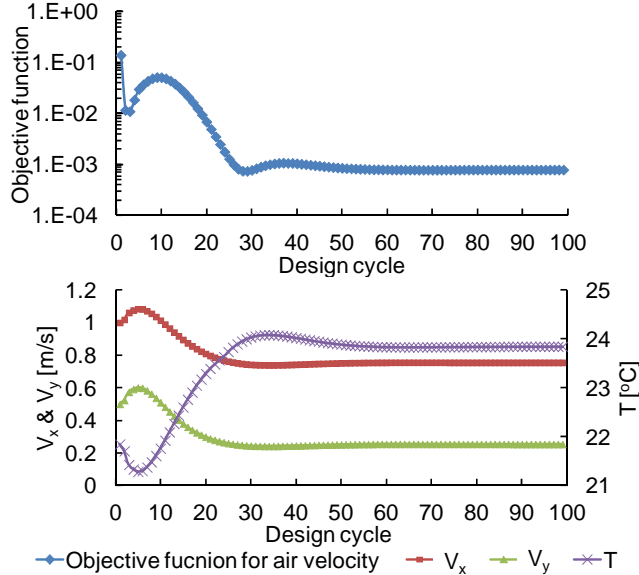
331 Since this was a non-isothermal case, the adjoint method also solved the energy equation.
332 Without iterations ($N_1=N_2=1$), the solution would have diverged as a result of highly
333 significant and sometimes unreasonable changes in the variables. Therefore, this study set
334 $N_1=N_2>1$ (see the solution flow chart) in the calculations in order to achieve a stable and
335 converged solution.
336

337 *3.2.1. Scenario 1: Using air velocity as the objective.* For this scenario, this study initialized
338 the inlet velocity and temperature as $V_x = 1 \text{ m/s}$, $V_y = 0.5 \text{ m/s}$, and $T = 6.85 \text{ °C}$ as Case 1a and
339 $V_x = 1 \text{ m/s}$, $V_y = 0.5 \text{ m/s}$, and $T = 21.85 \text{ °C}$ as Case 1b. Furthermore, this investigation used
340 $N_1=N_2=100$ for each design cycle and conducted 100 design cycles. Figure 10 shows that the
341 objective function was as small as 10^{-3} at the end of the calculation, indicating that an optimal
342 design had been reached. However, the two initial conditions led to two different optimal inlet
343 conditions. Figure 10(a) shows a final inlet air velocity of $V_x = 0.563 \text{ m/s}$ and $V_y = 0.007 \text{ m/s}$
344 and a final inlet air temperature of $T = 14.85 \text{ °C}$. The final condition was very close to the true
345 inlet condition of $V_x = 0.57 \text{ m/s}$, $V_y = 0 \text{ m/s}$, and $T = 15 \text{ °C}$. However, Figure 10(b) shows a
346 final inlet condition of $V_x = 0.755 \text{ m/s}$, $V_y = 0.254 \text{ m/s}$, and $T = 21.85 \text{ °C}$, which is quite
347 different. Because only the velocity field was used as the design objective, multiple optimal
348 solutions could exist.
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(a) Case 1a with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 6.85^\circ\text{C}$



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(b) Case 1b with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 21.85^\circ\text{C}$

Figure 10. Changes in V_x , V_y , and T at the inlet and the objective function with the number of design cycles, with partial flow field as design objective.

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As in the isothermal case, this study also conducted forward CFD simulations with final inlet air velocity and temperature determined by the adjoint method. Figure 11 compares the computed velocity profiles at mid-cavity ($x = 0.52$ m) with that using the exact inlet condition of $V_x = 0.57$ m/s, $V_y = 0$ m/s, and $T = 15^\circ\text{C}$. It can be seen that the two final inlet conditions had almost the same velocity profiles as the design objective.

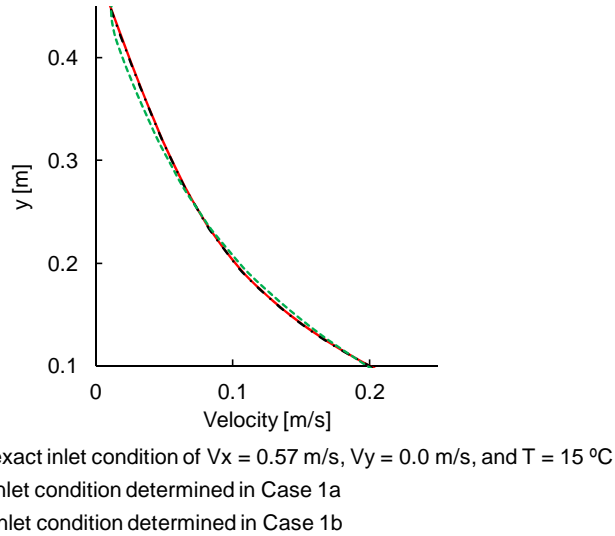
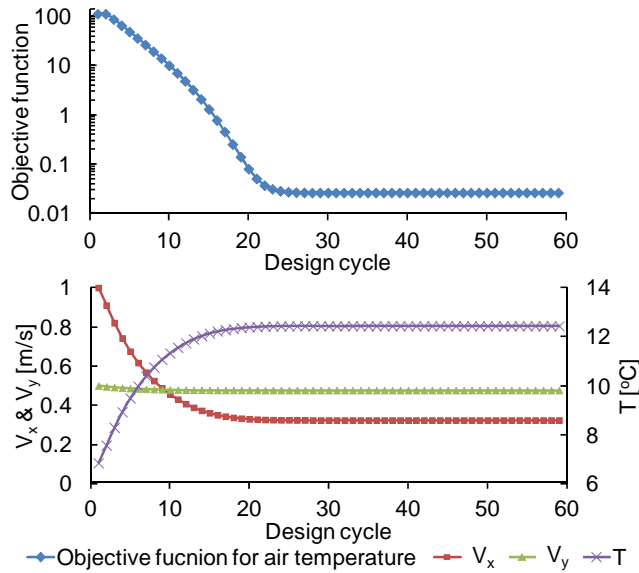


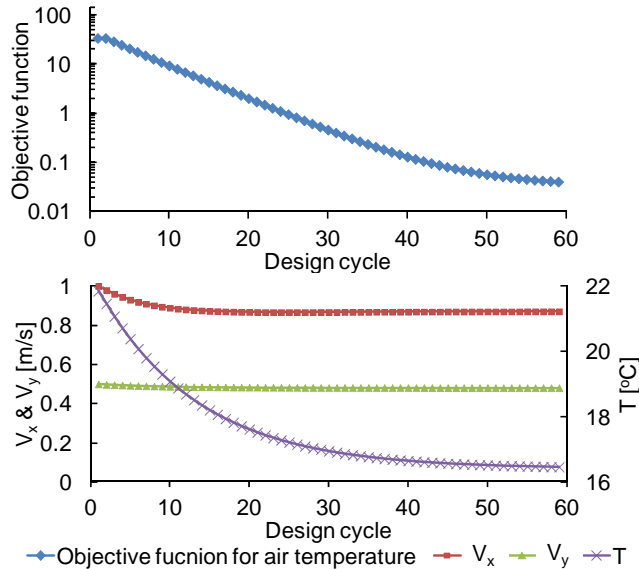
Figure 11. Comparison of the design objective (velocity profiles) determined by the adjoint method and that determined by the specified inlet condition of $V_x = 0.57$ m/s, $V_y = 0$ m/s, and $T = 15$ °C at $x = 0.52$ m.

3.3.2. *Scenario 2: Using air temperature as the objective.* Since it is much harder to obtain a converged result after adding the energy equation into the adjoint method, N_1 and N_2 were set at 5000. This study again initialized the inlet velocity and temperature as $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 6.85$ °C as Case 2a and $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 21.85$ °C as Case 2b. Figure 12 shows that, the objective function decreased gradually to about 0.02 in 60 design cycles. Then the corresponding average temperature difference between the temperature design objective and the calculated temperature distribution in the lower part of the mid-cavity was about 0.01 K. However, the optimal inlet air conditions are $V_x = 0.324$ m/s, $V_y = 0.477$ m/s, and $T = 12.44$ °C for Case 2a and $V_x = 0.870$ m/s, $V_y = 0.482$ m/s, and $T = 16.47$ °C for Case 2b, which are quite different from the true value of $V_x = 0.57$ m/s, $V_y = 0$ m/s, and $T = 15$ °C. This study also tried some other initial conditions, and the calculation always approached optimal solutions that differed from the true value, although the objective function became as small as 10^{-2} . Because different inlet conditions can lead to similar temperature distributions in the lower part of the mid-cavity, multiple optimal solutions are not a complete surprise to us.



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(a) Case 2a with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 6.85^\circ\text{C}$



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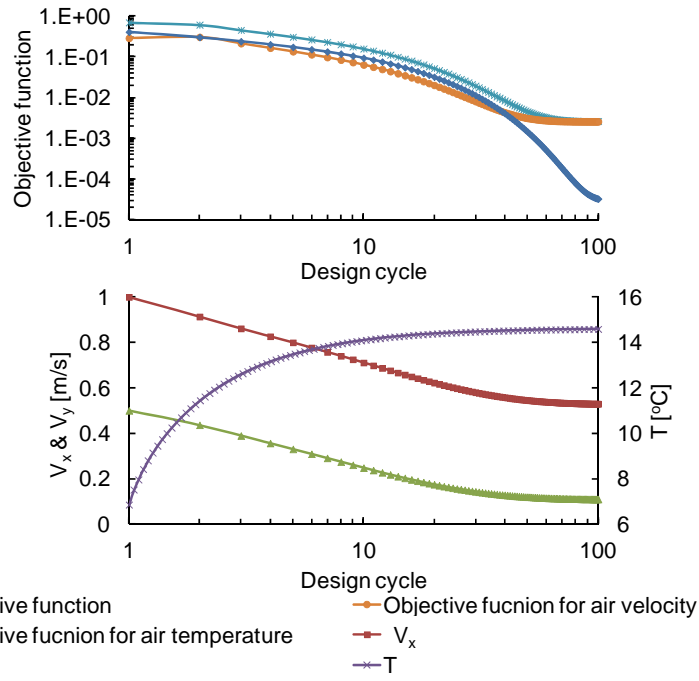
(b) Case 2b with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 21.85^\circ\text{C}$

Figure 12. Changes in V_x , V_y , and T at the inlet and objective function with the number of design cycles, with partial temperature field as design objective.

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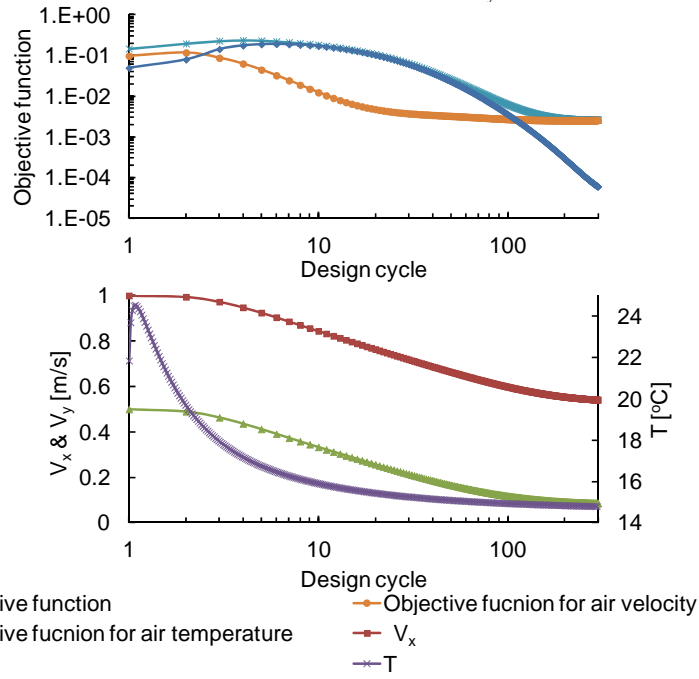
393 **3.3.3. Scenario 3: Using air velocity and temperature as the objective.** The design objective in
 394 Scenario 3 is to satisfy the air velocity and temperature profile in the lower part of the mid-
 395 cavity. This study again used an initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T =$
 396 6.85°C as Case 3a, and a condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 21.85^\circ\text{C}$ as Case 3b.
 397 N_1 and N_2 were set at 1000, which is a trade-off between the convergence of the calculations
 398 and computing effort. For each condition, this study calculated no more than 400 design
 399 cycles. Figure 13 shows that the final thermo-fluid boundary condition at the inlet for Case 3a
 400 was $V_x = 0.528$ m/s, $V_y = 0.109$ m/s, and $T = 14.63^\circ\text{C}$, and for Case 3b it was $V_x = 0.537$, V_y
 401 $= 0.084$ m/s, and $T = 14.68^\circ\text{C}$. The two final inlet conditions agree well with the true
 402 condition at the inlet as $V_x = 0.57$ m/s, $V_y = 0$ m/s, and $T = 15^\circ\text{C}$. It seems that the optimal

403 solution was unique when both the air velocity and temperature profiles were specified as the
 404 design objective.
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(a) Case 3a with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 6.85^\circ\text{C}$



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(b) Case 3b with initial inlet condition of $V_x = 1$ m/s, $V_y = 0.5$ m/s, and $T = 21.85^\circ\text{C}$

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Figure 13. Changes in V_x , V_y , and T at the inlet and design objective with the number of design cycles, with partial flow and temperature fields as design objective.

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Figure 13 also shows that the objective function for air velocity became 10^{-3} and that for air temperature became 10^{-2} . The corresponding average velocity in the lower part of the mid-

416 cavity differed by only 0.003 m/s from the design objective, and the average air temperature
417 differed by only 0.01 K from the design objective.

418

419 **4. Discussions**

420

421 In the isothermal case, within 1 iteration/cycle \times 2000 cycles, the adjoint method could
422 find the optimal inlet air velocity. The calculation time was roughly twice that required by
423 forward CFD simulation for 4000 iterations (no internal iteration) in solving the flow.
424 However, in Scenario 3 of the non-isothermal case, the adjoint method could also find the
425 optimal inlet conditions in 1,000 iterations/cycle \times 400 design cycles. The more complex flow
426 can increase the computing effort by one or two magnitudes.

427 In addition, the more design objectives there are, such as in Scenario 3, the lower the
428 likelihood that multiple solutions will occur. It is possible that if too many design objectives
429 are specified, then no solution can be obtained.

430 This study aimed to verify the applicability of the adjoint method in the optimal design of
431 indoor environment, so the design variables were only the inlet air velocity and temperature.
432 The former investigations [10, 11] showed that this method should work with more design
433 variables. However, the design variables in this study are of different types (velocity and
434 temperature) that are different from the application of this adjoint in other areas. This study
435 verified the inverse identification of design variables in different types.

436 This is our first approach that inversely designs the indoor environment. The objective
437 functions were only the partial air velocity and temperature profiles, the design variables were
438 only the inlet air velocity and temperature, and the cases for validation were two-dimensional.
439 We are rather happy to have achieved the goals set. Based on the results obtained in this
440 study, our future work will continue on the following three aspects: (1) more design variables
441 such as inlet location and size, and the interior furnishings, etc.; (2) expansion to three-
442 dimensional and more challenging cases such as an office or an aircraft cabin; and (3) more
443 challenging design objectives, such as thermal comfort, indoor air quality, and energy
444 efficiency, etc.

445

446 **5. Conclusions**

447

448 This investigation developed an adjoint method and implemented it in OpenFOAM to
449 determine the optimal thermo-fluid boundary conditions for designing the best indoor
450 environment. By applying the method to solve the inlet conditions with air velocity and/or air
451 temperature in rooms as the design objective, the inlet conditions could be inversely
452 identified.

453 For the isothermal case, this study used a velocity profile in the lower part of the room
454 computed by a forward CFD simulation as the design objective. The results showed that this
455 adjoint method could accurately find the optimal inlet air velocity by using different initial
456 inlet conditions. However, the calculations with different initial inlet air conditions led to
457 different optimal inlet air conditions, which implies the existence of multiple solutions.

458 For the non-isothermal case, when only the air velocity profile or only the air temperature
459 profile in the lower part of the mid-cavity was used as the design objective, the calculation led
460 to multiple solutions. When both the air velocity and temperature profiles were used as the
461 design objective, the calculations with different initial inlet air conditions found a unique
462 solution for the inlet condition.

463 **Nomenclature**

464 *Symbol definition*

465	D	rate of strain tensor
466	\bar{g}	gravity vector, $\text{m}\cdot\text{s}^{-2}$
467	J	objective function
468	L	augmented objective function
469	\bar{n}	unit vector in the normal direction
470	N	iteration numbers
471	p	pressure, Pa
472	Re	Reynolds number
473	S	Navier-stokes equations vector form
474	T	temperature, °C
475	TI	turbulence intensity
476	V	velocity, vector, $\text{m}\cdot\text{s}^{-1}$
477	x, y	index of coordinates

478

479 ***Subscripts***

480	0	design objective
481	a	adjoint parameter
482	fl	value at the floor
483	i	component of a vector
484	inlet	value at the inlet
485	n	normal component
486	old	value at prior design cycle
487	op	operating value
488	t	tangential component
489	wall	value at the wall
490	x	component in the x direction
491	y	component in the y direction

492

493 ***Superscripts***

494	i	component of a vector
495	T	transpose

496

497 ***Greek symbols***

498	α	positive constant
499	β	positive constant
500	γ	thermal expansion coefficient
501	δ	variation
502	ε	positive constant
503	θ	design domain
504	κ	effective conductivity
505	λ	positive constant
506	ν	effective viscosity
507	ξ	positive constant
508	Γ	effective diffusivity
509	Ω	flow domain

510 **Acknowledgements**

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