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TR2022-077 August 06, 2022

Abstract

Motivated by attempts to reduce the spread of disease during the current pandemic, we investigate modifications to heating, ventilation, and air-conditioning (HVAC) systems. Our aim is to minimize airborne droplet transport, modelled as an advection-diffusion PDE, through optimization of ventilation and management of airflow patterns within the built environment. Thus, we consider the optimization of turbulent flows within enclosed environments using the direct-adjoint-looping (DAL) optimization. We use the incompressible Reynolds-averaged Navier-Stokes (RANS) equations, derive the corresponding adjoint equations and solve the resulting sensitivity equations with respect to boundary conditions. For validation, we solve an inverse-design problem, for which we recover known globally optimal solutions. We then solve the minimal mixing problem for a passive scalar in a region of interest, as representative of potentially infected droplet transfer between occupants. It is shown that the exposure time of occupants reduce drastically by optimizing merely the direction of the inlet velocity.

International Conference on Building Energy and Environment (COBEE) 2022

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Airflow Optimization to Prevent Transmission of COVID-19

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Keywords: Adjoint analysis, COVID-19, PDE-constrained optimization, Turbulent flows, Optimal design and control

SUMMARY

Motivated by attempts to reduce the spread of disease during the current pandemic, we investigate modifications to heating, ventilation, and air-conditioning (HVAC) systems. Our aim is to minimise airborne droplet transport, modelled as an advection-diffusion PDE, through optimization of ventilation and management of airflow patterns within the built environment. Thus, we consider the optimization of turbulent flows within enclosed environments using the direct-adjoint-looping (DAL) optimization. We use the incompressible Reynolds-averaged Navier-Stokes (RANS) equations, derive the corresponding adjoint equations and solve the resulting sensitivity equations with respect to boundary conditions. For validation, we solve an inverse-design problem, for which we recover known globally optimal solutions. We then solve the minimal mixing problem for a passive scalar in a region of interest, as representative of potentially infected droplet transfer between occupants. It is shown that the exposure time of occupants reduce drastically by optimizing merely the direction of the inlet velocity.

INTRODUCTION

An air-conditioner induced Covid-19 outbreak, e.g., by asymptomatic patients in restaurants or other enclosed indoor spaces is reported in peer-reviewed studies in China and also by CDC, which exposes our vulnerability to future outbreaks linked to ventilation in public spaces [1]. Adequate building ventilation in hospitals and public spaces is, therefore, a crucial factor to contain the disease, to avoid the potential lockdown situations in future, and to reduce the chance of subsequent waves of outbreaks. In the past few decades, the field of architectural fluid dynamics has seen considerable advances in the form of better theoretical understanding of buoyancy-driven indoor flows, novel experimental techniques, and advanced numerical methods [2]. Nonetheless, while existing ventilation and space-conditioning systems are designed to manage thermal comfort in occupied spaces, they do not address current needs of reducing the spread of disease and contaminants. There is a rising interest in using techniques in the field of optimal design and control of flow within the built environment to also include the task of disease prevention indoors [3]. The complicated dynamics of airflow within the built environment, and its interaction with occupants, building, and the exterior, necessitate a systematic approach to accomplish this task.
There are various methods to determine air velocity, temperature, relative humidity, and contaminant concentration in a room, such as computational fluid dynamics (CFD), analytical models, and experimental measurements. However, such methods most often employ a trial-and-

error process to design HVAC systems that achieve desired conditions in the built environment. This process can become computationally intractable for large number of design variables, rely on domain expertise, and does not come with a mathematical guarantee for the optimality.

Recently, many researchers have attempted to use optimization methods such machine-learning (ML) based methods [4], genetic algorithm (GA) method [5] and reduced order modeling [6], which come with many promises. However, such methods still are very expensive in terms of training the models and lack appropriate physical interpretation.

The adjoint method has long been identified as the method of choice for optimization in fluid mechanics. Indoor airflow optimization is aimed at obtaining optimal boundary actuation (either steady or time-varying) that leads to desired airflow temperature, velocity, or concertation distribution characteristics in the domain of interest. In the past decade, application of systematic optimization and control to indoor airflow has been gaining attention. A parallel but related recent development is the use of nonlinear adjoint optimization techniques to find optimal, i.e., minimal energy, perturbations that lead to turbulence in canonical flows.

In our previous work [7, 8], we formulated and solved a model test-case problem of optimal design to determine steady and transient inlet velocity and temperature that optimize a certain cost functional related to achieving a desired temperature distribution in part of a room using the Direct-Adjoint-Looping (DAL) method. That study focused on the fully turbulent mixed-convection regime, resulting from the presence of a line heat source in addition to forced conditioned air from the inlet. Since DNS/LES based numerical optimization is not feasible with reasonable computing resources, we employed Reynolds-Averaged Navier-Stokes (RANS) models to account for interaction between the mean-flow and turbulent eddies. We validated the numerically computed optimal solutions with those obtained by optimizing experimentally-verified analytical reduced-order models for the same problem.

In this paper, we build up on our previous works by extending the results for thermal comfort maximization (plus energy consumption minimization) to the problem of minimization of virus concertation. In this spirit, the active scalar temperature is replaced with passive scalar as representative of disease transport. We use exposure time as a metric to quantify the performance of optimal ventilation on the discharge of a hypothetical concertation. The rest of the paper is organized as follows. In Section 2, we discuss the model and describe the schematic of the problem. We also formulate the optimal control problem and discuss the implementation of the DAL method to solve such problems. In Section 3, we discuss the results of the optimal design problems. In Section 4, we provide conclusions and sketch out directions for future research.

METHODS

This optimization problem involves buoyancy-driven airflow in a 2D room. A schematic for the problem domain D is shown in Fig. 1. The height and the length of the room are denoted by H and L, respectively. We divide the room into two hypothetical regions: a 'contagious zone', which contains the source of virus of contamination, on the left with length ℓ_1; and a 'safe zone', for which the occupants are assumed to be virus-free, on the right of the room. Each zone has two inlets and one outlet, which are indexed as shown in Fig. 1. A prescribed inflow is provided, for example, by an air conditioning unit or a mechanical fan. The inlet velocity is $V_{in,i}$ with $i \in \{1,2,3,4\}$ indicating the index of the inlet. For instance, $V_{in,1}$ is the velocity boundary condition of inlet 1 with horizontal and vertical components of $V_{in,1}^{x}$ and $V_{in,1}^{y}$. The design variables are taken to be the magnitude and direction of the inlet velocity. Typical Reynolds number in our experiments are *15000<Re<75000*.

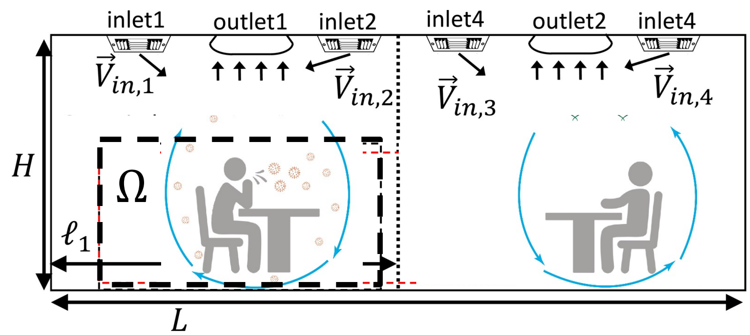

Figure 1. Schematic of the problem. The goal is to reduce concentration in the region of interest Ω *(the occupants in the schematic are for demonstration purpose only; in our preliminary results we only consider empty spaces and assume the source of contamination is on the left side).*

The test case was first motivated by application to 'targeted' cooling of the occupied zones in large open areas within a built environment. Such a zone cooling approach potentially leads to a decrease in the energy consumption while maintaining thermal comfort for the occupants. The region of interest, denoted by Ω, is a rectangular region that extends from $x = 3\text{m}$ to $x = 5\text{m}$ in the horizontal direction and from the floor to a height of $y = 1.5\text{m}$, to mimic a typical occupancy height in the contagious zone.

The turbulent flow for a passive scalar is governed by (using Einstein notation)

$$\begin{aligned} &\frac{\partial v_j}{\partial x_j} = 0 \\ &\frac{\partial v_i}{\partial t} + \frac{\partial v_i v_j}{\partial x_j} + \frac{\partial p}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\frac{1}{Re}\frac{\partial v_i}{\partial x_j}\right) = 0 \\ &\frac{\partial C}{\partial t} + v_j\frac{\partial C}{\partial x_j} - S - \frac{\partial}{\partial x_j}\left(\frac{1}{Sc}\frac{\partial C}{\partial x_j}\right) = 0 \end{aligned} \tag{1}$$

with $\boldsymbol{v}, p, C$ as ensemble-averaged velocity, pressure and concentration, respectively. We define $Re = \frac{V_{ref}L_{ref}}{\nu_{eff}}$ $Sc = \frac{\nu_{eff}}{D_{eff}}$ with ν_{eff} and D_{eff} are effective viscosity and diffusivity. We assume iso-thermal flow in this study. Boundary conditions are Dirichlet at inlet and walls (no-slip) for velocity, Naumann (zero gradient) at outlet for velocity, Naumann at inlet and walls for pressure, and Dirichlet (homogenous) for pressure at outlet. The inlet velocity magnitude and height H are chosen as reference values. For concentration C, we assume Naumann boundary condition on all surfaces. S is the source point, which resembles the source of coughing at the centre of contagious zone. The last line of Eq. 1 is a advection-diffusion transport for species, and here we assumed the transport of virus follows the same PDE [3, 9].

We now formally describe the optimization problem as

$$\min_{\vec{V}_{in}} J = \int_{\Omega} \int_{0}^{T} \dot{V}_b C \, dt \, d\forall \tag{2}$$

where J is the cost function, T is the time of integration, and $\dot{V}_b$ is the rate of inhalation (see Eq. 3 and 4 of [3] for more details). In this study, we normalize the concertation by its maximum value at the source such that the distribution of $C(x, y, t)$ is within $[0\ 1] \times T$ range.

We tackle the optimization problem by using the notion of the Lagrangian $\mathcal{L}$ to enforce the Boussinesq equations and constraints, as (in abstract form)

$$\mathcal{L} = \mathcal{J} + < \mathcal{P}, \mathcal{R} >, \tag{3}$$

where $\mathcal{P} = (v_a, p_a, C_a)$ is the vector of adjoint variables, and we use the notation $< f, g >= \int_{\Omega} fg \ d\forall$ is the so-called inner-product. The adjoint variables are Lagrange multipliers to enforce the state equations Eq. 1 and its boundary conditions. To ensure the (at least local) optimality of the solution, we choose the adjoint variables to enforce $\delta\mathcal{L} = 0$, where operator δ denotes variation. This idea is the core of the adjoint method. By enforcing that first order variations with respect to the state variables vanish at optimal solutions we obtain the adjoint equations as (for more details please see appendix of [7, 8])

$$\begin{gathered}
\frac{\partial v_{a,j}}{\partial x_j} = 0, \\
-\frac{\partial v_{a,i}}{\partial t} + v_{a,j}\frac{\partial v_j}{\partial x_i} - v_j\frac{\partial v_{a,i}}{\partial x_j} + C_a\frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_j}(\nu_{eff}\frac{\partial v_{a,i}}{\partial x_j}) + \frac{\partial p_a}{\partial x_i} = 0 \\
-\frac{\partial C_a}{\partial t} - v_j\frac{\partial C_a}{\partial x_j} - \frac{\partial}{\partial x_j}(\kappa_{eff}\frac{\partial C_a}{\partial x_j}) = -\dot{V}_b
\end{gathered} \tag{4}$$

We use the 'frozen turbulence' hypothesis in deriving Eq. 4. An assessment of the validity of this assumption has been carried out in [7]. The gradient of the cost function with respect to inlet velocity and temperature is obtained as follows.

$$\nabla_{V_{in}}\mathcal{J} = p_{a,in} - \nu_{eff}(n_i\partial/\partial x_i)v_{a,in}, \tag{5}$$

In order to update the inlet conditions, we apply a gradient descent method of the form:

$$V_{in}^{k+1} = V_{in}^{k} - \frac{\partial \mathcal{J}}{\partial V_{in}} \tag{6}$$

where superscript k denotes the number of iterations. We illustrate the iterative solution procedure schematically in Fig. 2, which shows the algorithm for the DAL method. The optimization begins with an initial guess for the design variables V_{in}. The set of `direct' or forward equations and adjoint equations are solved in a loop and the subsequent sensitivity calculation is used to obtain the next guess for the optimal design variables. This process is repeated until the convergence criterion for the cost functional is satisfied. Checkpointing method is used to address memory demands for implementation. For a complete details on derivation, verification, and validation of DAL please see our previous works and references therein [7, 8].

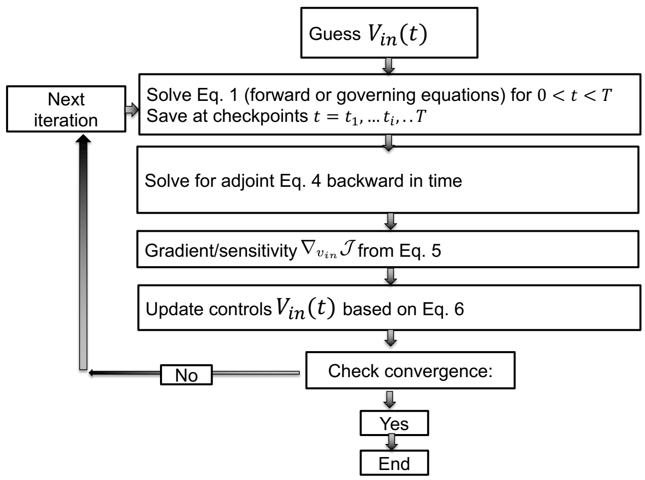

Figure 2. Flow chart for the Direct-Adjoint-Looping (DAL) method.

We use OpenFOAM [9], which is based on a finite-volume method with a collocated grid arrangement and offers object-oriented implementations that suit the employed continuous adjoint formulation. Pressure and velocity are decoupled using the SIMPLE algorithm [10] technique in the state/adjoint equations. For the convection terms, second order Gaussian integration is used with the Sweby limiter to account for propagation of density fronts, and numerical stability. For diffusion, Gaussian integration with central-differencing-interpolation is used. The advective terms in the energy equation are discretized using the second order upwind scheme of the van Leer method. The time integration was performed with the implicit Crank-Nicolson method, which is second-order bounded. The discretized algebraic equations are solved using the Preconditioned biconjugate gradient (PBiCG) method. The mesh sensitivity analysis is discussed is similar to [8].

RESULTS and DISCUSSION

We solve the optimization problem for three cases. Case 1 serves as a validation and it has a different cost function of the form $\min_{\vec{V}_{in}} J = \int_{\Omega} \int_0^T (V - V_d)^2 \, d\forall \, dt$. Here V_d is the desired velocity and is generated based on a prescribed velocity profile at the inlet, say V_{in}^d. Hence the optimal solution in this case is V_{in}^d and this class of problem is referred to as 'inverse problem'. We solve case 1 without considering the evolution of C. We set the initial guess as large perturbation of the optimal value, i.e., $V_{in}^{d} + \mathcal{O}\left(V_{in}^{d}\right)$. In other words, we non-trivially perturb the solution and verify if the DAL algorithm is able to recover the optimal solution at steady state. The results are shown in Figure 3, where the steady values of cost functions and gradients $\nabla_{V_{in}^{y}} J$ and $\nabla_{V_{in}^{x}} J$ for all 4 inlets are shown, as function of iterations k. As illustrated, by increasing the number of iterations, the cost function drops orders of magnitude and so do the absolute values of the gradients (sensitivities).

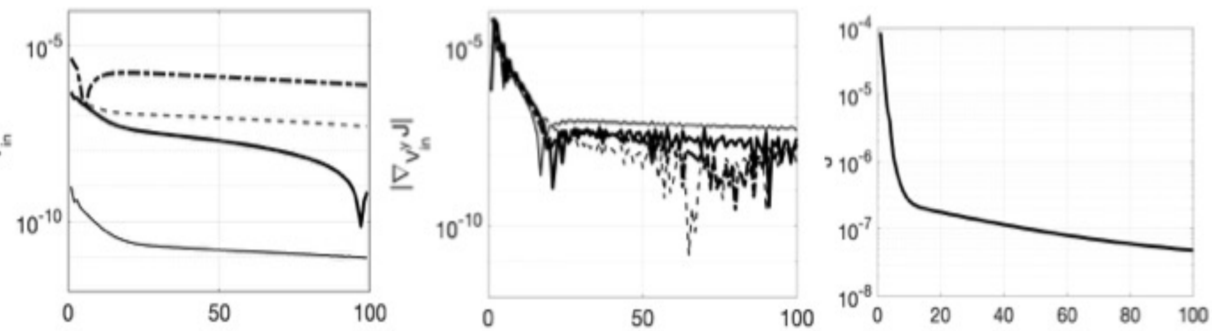

Figure 3. left) horizontal velocity sensitivity, middle) vertical velocity sensitivity, right) cost function for inverse problem based on DAL method. Values related to inlets 1, 2, 3 and 4 are denoted by thick solid, solid-dotted, dotted, thin solid lines, respectively.

In the next step, we consider the impact of optimization on the exposure time, i.e., the time interval during which the occupants are exposed to the virus. In case 2, we consider a non-optimal case, for which all the inlets are vertical, which is a typical scenario for ventilation. In case 3, however, we perform DAL and keep the volume flux at all the inlets equal to that of case 2 to show the importance of optimization on ventilation performance. Figure 4 shows the snapshots of the results for both cases at various times. The initial concentration and source term S is equal in both cases. As shown, by increasing time, the concentration of the non-optimal case becomes vanishing much faster than that of the non-optimal case. Such results are also confirmed in Figure 5, where the value of cost function of Eq. 2 is plotted for both cases as a function of time. This is an important result since such improvement is solely achieved by optimization the direction of velocity at the HVAC units and, hence, there is no additional energy consumption. It should be noted that, our DAL algorithm can take into account more constraints, e.g., on the range of direction or maximum value of V_{in}. Figure 5 confirms that C in Ω reaches 1% of its initial value in less than 10 units of time, while this never occurs for the non-optimal case in the time window considered. DAL, Similar to other gradient-based optimization methods, is seeking local minima. In this study, we used multi-start initial guess strategy to ensure the quality of optimization.

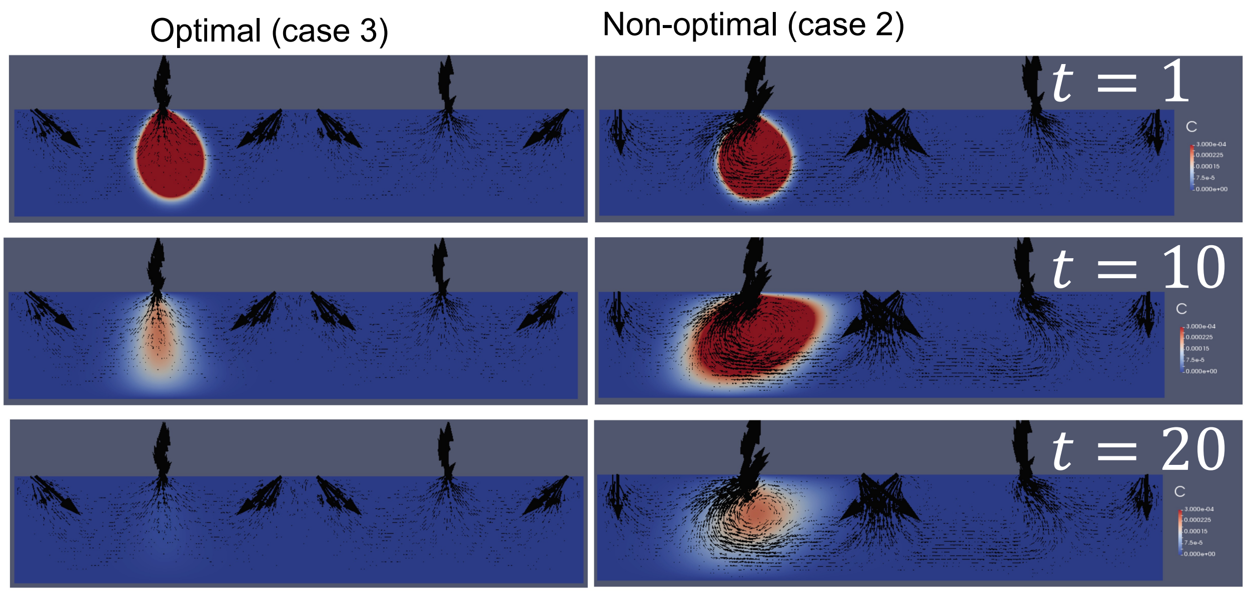

Figure 4. left column) Optimal, right column) non-optimal evolution of concentration C as a function of time. The spreading of the virus is represented by color-map red.

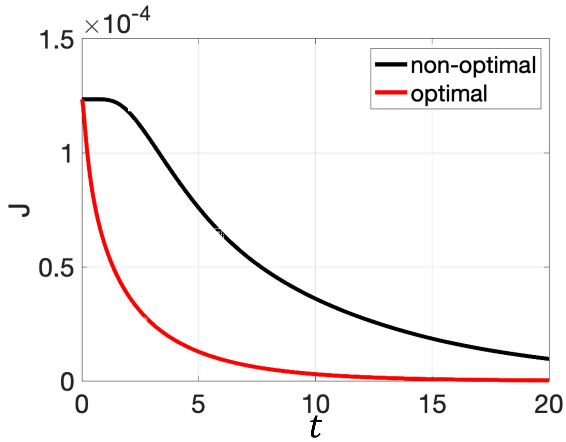

Figure 5. Evolution of cost function, as representative of the contamination in the region of interest Ω.

Finally, results of Figure 6 illustrate the optimal velocity pattern at steady state in the room. As shown for the optimal case, a formation of double counter-rotating vortices in the middle of the room are apparent. Such flow structures play an important role in minimizing the transport between the two zones of the room and acts like a virtual wall curtain that block the transport. An important outcome of this research is identification of such structures and their role in significantly reduction of the transport in the built environment.

CONCLUSIONS

We study the boundary optimization of turbulent flows using the DAL method. We model the impact of transport of disease, e.g., Covid-19, in the built environment based on a transport model, consistent with some other studies, e.g. [3]. The model has a stationary source term, but in future studies a moving source should be considered. Better understanding of the nature of spreading of the virus will lead to more sophisticated models for S. Moreover, other mechanisms such as evaporation should be considered in future. Two case studies demonstrate the numerical algorithm. In the first case study, we solve an inverse problem, for which we recover the optimal design. Next, we compared two scenarios, one with only vertical HVAC flow and the other with optimization on the direction. Our results clearly demonstrate the superiority of optimal case using DAL. The results of this paper are based on a 2D simulation. The next step is to consider a 3D setup with objects within the room as more realistic scenarios. This study can be seen as a proof of concept of applicability of adjoint method to prevent or reduce the spread of virus in the built environment.

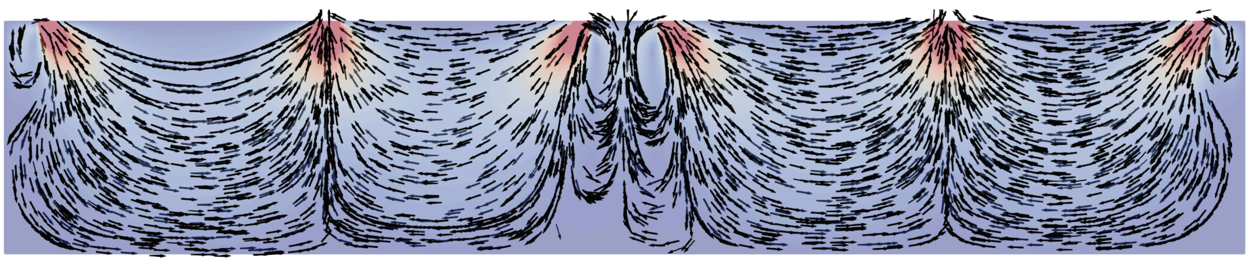

Figure 6. Streamlines (black) superposed on a colormap of the velocity magnitude for the optimal solution at steady state.

REFERENCES

[1] F.W. Moses, R. Gonzalez-Rothi, and G. Schmidt, "COVID-19 Outbreak associated with air conditioning in restaurant, Guangzhou, China, 2020", *Emerg Infect Dis*, vol. 26, pp. 2298-2298, 2020.

[2] Q. Chen, "Ventilation performance prediction for buildings: A method overview and recent applications", *Build Env,* vol. 44, pp. 848-858, 2009.

[3] V. Vuorinen, A. Mia, A. Mikko, A. Ville, A. Nina, A. Mikko, B. Nallannan et al. "Modelling aerosol transport and virus exposure with numerical simulations in relation to SARS-CoV-2 transmission by inhalation indoors.", *Safety Science,* vol. 130, p. 104866, 2020.

[4] W.A.Y. Mousa, W. Lang, T. Auer, and W.A. Yousef, "A pattern recognition approach for modeling the air change rates in naturally ventilated buildings from limited steady-state cfd simulations." *Energy and Buildings* vol. 155, pp. 54-65, 2017.

[5] Y. Xue, Z.J. Zhai, and Q. Chen, "Inverse prediction and optimization of flow control conditions for conned spaces using a cfd-based genetic algorithm." *Build Env* vol. 64, pp.77-84, 2013.

[6] S. Vijayshankar, S. Nabi, A. Chakrabarty, P. Grover, M. Benosman, "Dynamic mode decomposition and robust estimation: Case study of a 2d turbulent boussinesq flow". In 2020 American Control Conference (ACC), pp. 2351-2356. IEEE.

[7] S. Nabi, P. Grover, and C. Caulfield, "Adjoint-based optimization of displacement ventilation flow." *Build Env* vol. 124, pp. 342-356, 2017.

[8] S. Nabi, P. Grover, and C. Caulfield, "Nonlinear optimal control strategies for buoyancy-driven flows in the built environment." *Comp Fluid* vol. 194, p. 104313, 2019.

[9] OpenFOAM - the open source computational fluid dynamics toolbox, http://openfoam.com.

[10] S.V. Patankar, D.B. Spalding, "A calculation procedure for heat, mass and momentum transfer in threedimensional parabolic flows", *Int J Heat Mass* vol. 15, pp. 1787–1806, 1972.