Data-driven control of discrete-phase concentration in a vortex involved two-phase flow with optimized energy consumption

Zhang, Xingyu

2020

Zhang, X. (2020). Data-driven control of discrete-phase concentration in a vortex involved two-phase flow with optimized energy consumption. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/144249>

<https://doi.org/10.32657/10356/144249>

This work is licensed under a Creative Commons Attribution-NonCommercial 4.0 International License (CC BY-NC 4.0).

Downloaded on 26 Apr 2023 21:30:00 SGT

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

SINGAPORE

**DATA-DRIVEN CONTROL OF DISCRETE-PHASE
CONCENTRATION IN A VORTEX INVOLVED
TWO-PHASE FLOW WITH OPTIMIZED ENERGY
CONSUMPTION**

ZHANG XINGYU

**SCHOOL OF MECHANICAL AND AEROSPACE
ENGINEERING**

2020

**Data-driven control of discrete-phase concentration in a
vortex involved two-phase flow with optimized energy
consumption**

ZHANG XINGYU

School of Mechanical and Aerospace Engineering

A thesis submitted to the Nanyang Technological University
in partial fulfillment of the requirement for the degree of
Doctor of Philosophy

2020

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research is free of plagiarised materials, and has not been submitted for a higher degree to any other University or Institution.

13 /January/2020
Date

Zhang Xingyu
.....
ZHANG Xingyu

Supervisor Declaration Statement

I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

13/January/2020
Date

.....
Assoc. Prof. Li Hua

Authorship Attribution Statement

This thesis contains materials from one paper published and one paper in review in the following peer-reviewed journal, in which I am listed as an author.

Chapter 3 is published as X. Zhang, H. Li, Feasibility analysis for control of bioaerosol concentration at indoor corner via airflow from ventilation outlet with energy optimization, Journal of Cleaner Production (2019) 119289 (In press).

The contributions of the co-authors are as follows:

- A/Prof Li Hua and I worked together for the initial project direction.
- A/Prof Li Hua gave valuable advice and patient guidance during the project and edited the manuscript drafts.
- I prepared the manuscript drafts.
- I performed all the simulation work at the School of Mechanical and Aerospace Engineering in Nanyang Technological University in Singapore. I also analyzed the data.

Chapter 4 is under reviewed and potentially published as X. Zhang, H. Li, Neural-network-based control of discrete-phase concentration in a gas-particle corner flow with optimal energy consumption Computer & Mathematics with applications (in review).

The contributions of the co-authors are as follows:

- A/Prof Li Hua and I worked together for the initial project direction.
- A/Prof Li Hua gave valuable advice and patient guidance during the project and edited the manuscript drafts.
- I prepared the manuscript drafts.
- I performed all the simulation work at the School of Mechanical and Aerospace Engineering in Nanyang Technological University in Singapore. I also analyzed the data.

13/January/2020

Date

.....
Zhang Xingyu
Zhang Xingyu

Acknowledgments

I am sincerely grateful to my supervisor, Assoc. Prof Li Hua, for his continuous guidance support, encouragement, and suggestions during my ph.D study. What I have learned from him is not only about the research itself, but also about how to become an independent scholar.

I am also thankful to my Thesis Advisory Committee, Assoc Prof Duan Fei from NTU and Dr. Chen Ming from A*STAR, for their professional and invaluable suggestions.

My thanks also go to my friends, Dr. Liu Qimin, Dr. Goh Kekboon, Dr. Zhou Xiaoli, Dr. Yang Shiyu, Mr. Chen Xiao, Mr. Wang Yifeng, Dr. Zhan Zhixin, Mr He Lewei, Mr. Chen Kewei, and Ms. Chen Wanyu. I am heartily thankful for their assistance and encouragement during my ph.D study.

Table of contents

Acknowledgments	I
Table of contents	II
Summary	VI
List of figures.....	X
List of tables	XVI
List of symbols.....	XVIII
Chapter 1 Introduction	1
1.1 Background	1
1.1.1 Multiphase flow and application	1
1.1.2 Machine learning technique.....	4
1.1.3 Bioaerosol and indoor air quality	5
1.2 Motivation and objective	7
1.3 Thesis outline	10
Chapter 2 Literature review	12
2.1 Theoretical modelling of two-phase flow.....	12
2.1.1 Modelling of continuous phase dynamics	13
2.1.2 Modelling of discrete phase dynamics	17
2.1.3 Modelling of interaction between two phases	18
2.2 Control strategies for two-phase flow	20
2.2.1 Control of continuous-phase pattern.....	20
2.2.2 Control by structure design.....	21
2.2.3 Controller design based on a reduced-order model	22
2.3 Machine learning-based modelling and control of two-phase flow	23
2.3.1 Machine-learning based fluid mechanics	23
2.3.2 Machine-learning based two-phase flow	27
2.3.3 Machine-learning based control methods.....	28
2.4 Indoor bioaerosols dynamics	30

2.4.1	Modelling and experiment of indoor bioaerosol dynamics	30
2.4.2	Impact on growth and release of indoor bioaerosols	31
2.4.3	Impact on bioaerosol dynamics in airflow	33
2.5	Remarks	34
Chapter 3	Development of control strategy of particle concentration for two-phase potential corner flow with optimized energy consumption	37
3.1	Problem statement	38
3.2	Modeling of two-phase potential corner flow	40
3.2.1	Flow pattern at corner	40
3.2.2	Particle dynamics	44
3.2.3	Nondimensionalization and numerical flowchart	48
3.3	Validation of two-phase flow model	51
3.4	Simulation configuration, results and discussions	54
3.4.1	Simulation configuration for case studies	55
3.4.2	Case study I: Suspending particle dynamics without control initially in different regions at corner	64
3.4.3	Case study II: Suspending particle dynamics without control by different initial distributions at corner	68
3.4.4	Case study III: Optimized energy control for bioaerosols initially suspended at indoor corner with different distributions	70
3.4.5	Case study IV: Optimized energy control for bioaerosols released from the partial ceiling and wall	77
3.4.6	Case study V : Optimized energy control for bioaerosols/detergents released from ventilation outlet	82
3.4.7	Recommended guidelines for optimal operation conditions	89
3.5	Remarks	91

Chapter 4	Development of Neural Network Model Predictive Control (NN-MPC) controller of particle concentration for two-phase laminar corner flow with optimized energy consumption....	93
4.1	Problem statement	94
4.2	Modeling of gas-particle laminar corner flow	95
4.2.1	Gas-particle corner flow model	95
4.2.2	Definition of recirculation zone.....	97
4.3	Development of NN-MPC controller	99
4.3.1	NN leaning of recirculation zone characteristics.....	100
4.3.2	Design of MPC controller.....	101
4.4	Validation of the two-phase flow model	103
4.5	Simulation configuration, results and discussions	106
4.5.1	Simulation configuration of gas-particle two phase flow.....	107
4.5.2	Case study I: Particle dynamics without control at corner	109
4.5.3	Case study II: Minimization of residual bioaerosol concentration at the corner with optimized energy consumption via NN-MPC controller	113
4.6	Remarks.....	116
Chapter 5	Data-driven control of particle concentration within a turbulent corner flow via proportional-integral-derivative (PID) controller with optimized energy consumption	118
5.1	Problem statement	118
5.2	Modelling of gas-particle turbulent corner flow	119
5.2.1	Dynamics of turbulent gas phase.....	120
5.2.2	Dynamics of bioaerosols	123
5.3	Design of PID controller for gas-particle turbulent corner flow	125
5.3.1	System identification by transfer function models	126

5.3.2	PID controller design by the reduced model	127
5.4	Validation of two-phase flow model with backward facing step experiment	129
5.5	Simulation configuration, results and discussions	134
5.5.1	Simulation configuration	135
5.5.2	Case study I: Suspending particle dynamics without control at corner	137
5.5.3	Case study II: Control of residual particle concentration at indoor corner with optimized energy consumption via PID controller .	145
5.6	Remarks.....	151
Chapter 6	Conclusions and Recommendations	154
6.1	Conclusions from present work.....	154
6.2	Recommendations for future work.....	158
References		164
Publications arising from the thesis		179

Summary

Control of the discrete-phase (e.g. particles or bioaerosols) concentration in a two-phase flow has a wide range of attractive applications in engineering. However, it is difficult to achieve the objective concentration with optimized energy consumption, due to the complex flow of the fluidic phase and its effect on the discrete phase, especially in a single-inlet fluid field with fixed geometric structure. Moreover, the limits of computational ability constrain the design of control algorithm to achieve an optimized discrete-phase concentration in a two-phase flow.

Therefore, this thesis aims to develop novel methods systematically to control the discrete-phase concentration in a two-phase flow, by modulating the flow pattern via the existing vortex in the fluid field, with optimized energy consumption for control actuation. The proposed methods are conducted to control the bioaerosol concentration at indoor corner, defined as the area around ceiling edges, in order to improve the indoor air quality that is very important to resident health. Three major academic achievements from the present research are summarized respectively as follows.

The first achievement of the present research provides a feasibility analysis for control of bioaerosol concentration at an indoor corner, through airflow from ventilation outlet with optimized energy consumption. In the proposed control strategy, a gas-particle flow model with a chaotic moving vortex is developed to simulate the bioaerosol movement at an indoor corner via the Eulerian-Lagrangian scheme. In this model, the flowrate of the inlet fresh or air-conditioned air is tuned by a flowrate controller, which is installed at ventilation

outlet or inside ventilation duct, in order to control the vortex trajectory. A residual concentration is defined as the ratio of the residual number of densely released particles at the corner to the area of the corner, in order to indicate the probability of bioaerosol movement, which is released sparsely and randomly by a microorganism in a real-world situation. The control strategies are then developed to optimize residual bioaerosol concentration and energy consumption by the orthogonal scheme. Based on the simulation results, a small variation of the airflow rate from the ventilation outlet contributes to reduction of the residual concentration of bioaerosols that are originally released from the corner, or to increase of the residual concentration of detergents that are released from the ventilation outlet. It is thus concluded that a Pulse Width Modulation controller, with low amplitude, proper duty factor, period and time delay, is more energy efficient to improve the local indoor air quality.

The second achievement is the development of a machine-learning based method for control of local bioaerosol concentration, via the forced laminar corner flow with optimal energy efficiency at an indoor environment. A recirculation zone determined by the inlet flow rate traps particles partially with one or more vertexes around the corner. The profile of the recirculation zone is then determined mathematically, by the minimum net mass flux principle with a grid search technique. After that, the variation of the recirculation zone profile is learned via Neural Network (NN), in which dataset is collected from the simulation by the Eulerian-Lagrangian scheme. Moreover, a model predictive control (MPC) algorithm is implemented to achieve an optimal profile of the recirculation zone with optimal energy consumption, based on the linearized NN model. Finally, the proposed NN-MPC is employed to improve the local

bioaerosol environment at indoor corner through a flow-rate-controllable air inlet located at ceiling.

The third achievement is an extension to turbulent from laminar flow mentioned above, for modelling of the continuous phase dynamics in two-phase corner flow, in order to control the discrete-phase concentration with optimal energy efficiency. The extended turbulent two-phase corner flow model is carried out by computational fluid dynamic (CFD) simulations, in which the turbulent effect is simulated by Menter's Shear Stress Transport (SST) $k - \omega$ model, and the particle phase simulated by Eulerian-Lagrangian scheme. A great agreement is achieved against experimental data of a backward facing step, with an error of 12.2% for the maximum negative velocity in the recirculation zone. The simulation results are then used as input/output data for system identification by linear transfer function models, describing the relationship between inlet flowrate and particle concentration. A proportional-integral-derivative (PID) controller is tuned to minimize the residual particle concentration with optimized energy consumption for control. Simulation results demonstrate highly effective controllability of PID controller, reducing maximumly 24.16% of the particle concentration compared with natural ventilation (zero control). In addition, the efficient energy consumption is discussed among different sets of controller parameters, based on the requirements of the energy and residual particle concentration. However, there is still a space for improvement of the controller based on a better system identification algorithm, since it is difficult for the linear transfer function model to capture the nonlinear dynamics in the turbulent two-phase flow. Moreover, it is easy and fast for PID control to tune with effective

improvement of particle removal, although other control methods probably achieve better control performance.

List of figures

Figure 1.1 Schematics of (a) a fluidized bed reactor to split photocatalytic water [4], (b) spraying process of an effervescent atomizer [5, 6], and (c) diffusion process of indoor airborne particulate pollutant [7]	2
Figure 1.2 Thesis outline.....	11
Figure 3.1 Schematic of the indoor corner with pollution of bioaerosols.....	38
Figure 3.2 Schematics of corner flow with bioaerosols, (a) bioaerosols released from partial ceiling and wall, (b) bioaerosols or detergents released from ventilation outlet.....	40
Figure 3.3 Computational flowchart	51
Figure 3.4 Comparison of present theoretical simulation with published theoretical and experimental works [170] for particle distribution in a single Rankine point vortex	54
Figure 3.5 Comparison of trajectory of vortex centres subject to zero control input and two representative control inputs	62
Figure 3.6 Schematic flow chart of controller design to optimize residual particle concentration in a gas-particle corner flow via orthogonal design ..	64
Figure 3.7 Evolution of (a) different forces imposed on a single particle, and (b) particle trajectory in boundary layer	65
Figure 3.8 Division of the particle suspending area.....	66
Figure 3.9 Evolution of particle movement in Zone 5 at (a) $\tau = 0.5$, (b) $\tau = 2.3$, (c) $\tau = 5$	66
Figure 3.10 Evolution of particle movement in Zone 7 at (a) $\tau = 0.5$, (b) $\tau = 2.3$, (c) $\tau = 5$	67

Figure 3.11 Variation of residual particle concentration with dimensionless time τ	67
Figure 3.12 Initial distribution of particles in moldy area	69
Figure 3.13 Variation of residual particle percentage with different initial distributions.....	69
Figure 3.14 Energy consumption when the residual particle concentration is reduced to (a) 30%, (b)10%, and (c) 5% with HSF control inputs..	71
Figure 3.15 Selection of optimized HSF control input when residual particle concentration is reduced to 30%.	72
Figure 3.16 Selection of optimized HSF control input when residual particle concentration is reduced to (a) 10% and (b) 5%.....	73
Figure 3.17 Selection of optimized PWM control input with initially uniform distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.....	74
Figure 3.18 Selection of optimized PWM control input with initially normal distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.....	76
Figure 3.19 Selection of optimized PWM control input with initially normal distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.....	77
Figure 3.20 Evolution of movement for particle released from partial wall and ceiling with $\bar{e}_m = 0$ at (a) $\tau = 0$, (b) $\tau = 2$, (c) $\tau = 5$, (d) $\tau = 10$, (e) $\tau = 15$, (f) $\tau = 20$	78
Figure 3.21 Comparison of (a) residual concentration C_{ip} and (b) control efficiency γ_c subject to different HSFs with $\delta = 0$	79

Figure 3.22 Variation of loss function Φ with different control inputs at different weight factors (a) $\lambda_2 = 0.8$, (b) $\lambda_2 = 1$, and (c) $\lambda_2 = 1.2$..80	
Figure 3.23 Evolution of movement for particles released within ventilation outlet with $\bar{e}_m = 0$ at (a) $\tau = 0.5$, (b) $\tau = 2$, (c) $\tau = 5$, (d) $\tau = 10$, (e) $\tau = 15$, and (f) $\tau = 20$ 84	
Figure 3.24 Comparison of (a) residual concentration C_{ip} and (b) control efficiency γ_c subject to different HSFs with $\delta = 0$ 85	
Figure 3.25 Variation of loss function Φ with different control inputs at different weight factors (a) $\lambda_2 = \lambda_3 = 0.8$, $C_\tau = 48$, (b) $\lambda_2 = \lambda_3 = 1$, $C_\tau = 48$ and, (c) $\lambda_2 = \lambda_3 = 1.2$, $C_\tau = 48$ 86	
Figure 4.1 Schematics of (a) the indoor corner with bioaerosol pollution, and (b) computation domain of the two-phase corner flow model 94	
Figure 4.2 Schematic flow chart of NN-MPC to optimize residual particle concentration in a gas-particle corner flow 99	
Figure 4.3 Structure of the RBF-NN with p input nodes, Q hidden nodes and single output node 101	
Figure 4.4 Schematic illustration of the two-phase point vortex flow model for validation..... 104	
Figure 4.5 Streamline and sediment position on rz plane of the two-phase point-vortex model at $t=50s$ 104	
Figure 4.6 Validation of the two-phase flow model against the experimental and theoretical work by Julien [170, 174] (a) averaged sediment concentration in radial direction from 30 to 50s (b) variation global error between simulation and experiments during 30 to 50s subject to different ranges of r/r_0 106	

Figure 4.7 Streamline of corner flow, evolution of particle distribution, and division of the recirculation zone at five representative time instants (a) $t=4s$, (b) $t=14s$, (c) $t=24s$, (d) $t=34s$, (e) $t=44s$	110
Figure 4.8 White-noise input for identification of the NN model	111
Figure 4.9 Variation of recirculation zone area $A[k]$ with sampling instant k	112
Figure 4.10 Variation of normalized particle concentration inside three different lines	113
Figure 4.11 Comparisons of predicted recirculation zone area (a), and corresponding relative simulation error (b) compared with NN and linearized NN models	115
Figure 4.12 Control input by NN-MPC algorithm.....	115
Figure 4.13 Comparison of particle concentration in different corner areas between natural ventilation (no control) and NN-MPC control	116
Figure 5.1 Schematics of (a) the indoor corner with bioaerosol pollution, and (b) computation domain of the two-phase turbulent corner flow model	119
Figure 5.2 Diagram of a feedback system containing a controller and an identified plant model	126
Figure 5.3 Schematic flow chart of controller design to optimize residual particle concentration in a gas-particle turbulent corner flow	128
Figure 5.4 Geometry of the backward facing step, with step height of 0.025 m, the inlet and outlet lengths of 1.25 m and 0.87m, respectively.	132
Figure 5.5 Velocity contour with streamlines around the backward facing step.	132

Figure 5.6 Comparison of particle velocity profiles from the present simulations with the experimental [92] and simulation (realizable $k-\varepsilon$) [90] studies	133
Figure 5.7 Comparison of the maximum negative particle velocity in recirculation zone behind step against the simulation and experimental results	134
Figure 5.8 Evolution of corner flow streamline and particle position at (a) $t=15s$, (b) $t=20s$, and (c) $t=25s$	138
Figure 5.9 Particle positions and velocities, at four different times for 1600 particles released at $t = 10s$, simulated with discrete random walk	139
Figure 5.10 Trajectories of neighboring particle releases, simulated with discrete random walk, with initial positions at (0.9, 0.8692), (0.9, 0.8731) and (0.9, 0.8769).....	140
Figure 5.11 Measured and averaged mean force imposed on particles within measurement triangle	140
Figure 5.12 Three excitation input singles for system identification.....	142
Figure 5.13 Comparison of residual particle concentration C_r by nature ventilation (1 m/s) and three excitation input signals, namely step of 1.2 m/s, chirp, and white noise	142
Figure 5.14 Comparison of residual particle reduction C_d by step of 1.2 m/s, chirp, and white noise excitation input signals against natural ventilation (1 m/s).....	143
Figure 5.15 Comparison of identified transfer function models excited by different (a) step of 1.2, (b) chirp, and (c) white noise excitation signals, with the relative residual particle concentration C_d by gas-particle turbulent flow simulations	144

Figure 5.16 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.1	149
Figure 5.17 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.125	150
Figure 5.18 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.15	151
Figure 6.1 Schematic flowchart for control of discrete-phase concentration by ML technique via comparison between potential flow and laminar flow	159
Figure 6.2 Schematic of 3D corner flow.....	160

List of tables

Table 1.1 Examples of multiphase flow [8]	3
Table 3.1 Input parameters of the two-phase model for motion of sediment particles in a Rankine point vortex	53
Table 3.2 Inputs of two-phase corner flow model	58
Table 3.3 Levels of control input parameters.....	60
Table 3.4 Design of control input HSF by orthogonal scheme.....	61
Table 3.5 Design of control input PWM by orthogonal scheme.....	61
Table 3.6 Average of loss function $\Phi_{n,avg}$ at each parameter level when $C_\tau = 30$ for Case Study IV.....	81
Table 3.7 Average of loss function $\Phi_{n,avg}$ at each parameter level when $C_\tau = 48$	87
Table 3.8 Summary of optimal operating conditions for Cases IV and V	90
Table 4.1 Input parameters for two-phase point vortex model for validation[170, 174]	103
Table 4.2 Inputs of the two-phase corner flow model.....	107
Table 4.3 Meshing details of grid convergence study for laminar corner flow	108
Table 4.4 Grid convergence study for laminar corner flow	108
Table 4.5 Average of particle concentrations in different areas by imposing natural condition and NN-MPC control input	116
Table 5.1 Parameters of SST turbulent model	123

Table 5.2 Parameters for validation against experiment.	130
Table 5.3 Parameter configuration for simulations	135
Table 5.4 Meshing details for grid convergence study	136
Table 5.5 Grid convergence study for turbulent corner flow	137
Table 5.6 PID controller parameters and corresponding step response performance	146
Table 5.7 Total energy consumption E_t , averaged residual particle reduction C_d , and terminal residual particle reduction C_d by different PID controllers	148

List of symbols

A	area of recirculation zone
d_p	particle diameter
D	diffusion coefficient
C	particle concentration
C_{ip}, C_r	residual particle concentration
C_d	relative residual particle concentration
C_p	ratio of density
e	coefficient of restitution
$e(t), e(\tau)$	control input signal
$E(t), E_{sig}$	energy consumption of control actuation
f	coefficient of friction
F_b	buoyancy
F_f	resistant force
F_g	Gravity
F_m	Magnus force
F_{LvdW}	London von der Waals force
F_p	pressure gradient force
F_{pfa}, F_{bla}	net force on particle in potential flow area and boundary layer
F_{sl}	Saffman lift force
h	Planck's constant
k_s	intensity of stagnation flow
k	turbulent viscosity
K_B	Boltzmann constant
M_p	mass of particle
l_c, l_o	length of corner zone side, distance of ventilation outlet to origin point
l_m, l_i	length of mouldy area, distance between two sources of particle
L_c	edge of recirculation zone
N, N_{ip}	amount of particle
O_c	particle measurement area
p	pressure of the fluid
p_c	pressure in vortex core

p_b	pressure in boundary layer
P, Q	Numbers of input and hidden nodes
P	interest position
P_n	position of vortex center
r_0	radius of vortex core
t	time
T	temperature
TF	transfer function
T_{on}	working duration of control input
T_s	period of pulse width modulation
t_h	holding time
u	velocity field of the fluid
U	velocity magnitude at the edge of boundary layer
u_{bx}, u_{by}	velocity in boundary layer of fluid at x and y direction
u_c	velocity at edge of vortex core
u_p	particle velocity vector
u_r	relative velocity
u_x, u_y	velocity of fluid at x and y direction
v	frequency
w_0	output bias
w_{pq}^i, w_p^o	weight matrixes of input layer and output layer
$\bar{X}$	root mean square particle displacement
γ_e, γ_e	energy and control efficiency
ξ_{ee}	averaged energy efficiency
ξ_{C_τ}	duration of particle concentration above a desired level
Γ	circulation of vortex
δ	time delay of pulse width modulation
η	duty factor of pulse width modulation
η_b	dimensionless velocity in boundary layer
θ	thickness of boundary layer
λ	weight factor
μ	dynamic viscosity
μ_T	turbulent viscosity

ν	kinematic viscosity
ρ_f	density of fluid
ρ_p	particle density
Φ	loss function
χ	step function
Ψ_s, Ψ_c	streamline of stagnation and controlled flows
Ψ_{oc}, Ψ_{nv}	streamline of overall flow and vortex pairs
Ψ_t	streamline of the fluid in Quadrants 2, 3 and 4
ω_d	angular velocity of particle

Chapter 1 Introduction

In this chapter, the background information relevant to multiphase flow dynamics, machine learning techniques, and indoor bioaerosol pollution is introduced, followed by the motivation and objectives of the present research work. The outline of the thesis is finally presented.

1.1 Background

The background of the present work is introduced in this section, consisting of three subsections, namely Multiphase flow and applications in Section 1.1.1, Machine learning in Section 1.1.2, and Bioaerosol and indoor air quality in Section 1.1.3.

1.1.1 Multiphase flow and application

In fluid mechanics, usually continuum fluidic materials are assumed, consisting of infinite fluidic particles. By the assumption, a flowing process is modelled by a group of closed equations based on the laws of mass, momentum, and energy conservations, with proper boundary and initial conditions. However, it is difficult to solve those equations theoretically, due to strong nonlinearity and multi-scaled turbulent vortices widely in fluid field. Therefore, several additional assumptions are required further for approximate numerical or theoretical solutions. One of the examples is the inviscid assumption that is applicable in flow region except boundary layer, if viscous force is much less than inertia in flow [1, 2]. By the inviscid assumption, Navier Stokes (NS) equation for incompressible fluid is simplified to the Euler equation. The inviscid flow model by Euler equation is further subdivided into rotational and irrotational flows, depending on the flowing characteristics of fluidic particle. On the other hand,

the viscous flow model is categorized into laminar and turbulent flows, depending on the flow status. Usually the two flows are distinguished by Reynolds number, in which a high Reynolds number leads to turbulence [1-3].

Figure 1.1 Schematics of (a) a fluidized bed reactor to split photocatalytic water [4], (b) spraying process of an effervescent atomizer [5, 6], and (c) diffusion process of indoor airborne particulate pollutant [7]

Table 1.1 Examples of multiphase flow [8]

Category	Examples
Gas-liquid flow	Bubbly flow
	Separated flow
	Gas-droplet flow
Gas-solid flow	Gas-particle flow
	Pneumatic transport
	Fluidized bed
Liquid-solid flow	Slurry flow
	Hydro-transport
	Sediment transport
Three-phase flow	Bubbles in a slurry flow
	Droplets/particles in gaseous flow

Another common flow phenomenon is multiphase flow, involving different phases simultaneously such as gas, liquid and solid states, generally categorized by gas-liquid, gas-solid, liquid-solid, and three-phase flows, or in the same phase but including two or more components such as liquid-liquid flow [9, 10]. The examples of each category are listed in Table 1.1 [8]. Compared with single-phase flow, multiphase flow is more complicated in modelling and control, due to difficult quantification of turbulence, with effect of mass, momentum and energy transfer between different phases [8, 11]. Therefore, approximate numerical solutions for multiphase flow are required by computational fluid dynamics (CFD) based computational methods, such as finite element method (FEM), finite volume method (FVM), spectral element methods (SEM), and boundary element method (BEM). CFD is often carried out by several commercial software, such as ANSYS Fluent, OpenFOAM, COMSOL Multiphysics, and Autodesk CFD, for simulation of multiphase flow involved engineering

processes, such as nano-manufacture [11], nuclear industry [12], combustion industry [13], chemical transportation [14], and environmental engineering [7]. For example, a liquid-particle flow is mixed in the fluidized bed reactor to produce hydrogen production via the reaction between solution and titanium dioxide particles, as illustrated in Figure 1.1(a) [4, 15]. For an effervescent atomizing process, small droplets are sprayed through a nozzle from a gas-liquid flow, mixed by the injected gas from the tube wall and the liquid from the tube entrance, as illustrated in Figure 1.1(b) [5, 6]. The diffusion of indoor airborne particulate pollutants is simulated by a gas-particle flow model for transportation dynamics of pollutants in a room, as shown in Figure 1.1(c) [7].

1.1.2 Machine learning technique

As well known, it is difficult for complex physical-based methods to achieve general solutions with desired accuracy. Instead of performing a theoretical analysis of the complex physical phenomenon, the approximate numerical solutions may be achieved by high performance computing. However, there still exists a trade-off between computational efficiency and accuracy. With the blossom of age of data in recent two decades, data-driven modelling methods (also called machine learning, artificial intelligence, or genetic algorithm) show great potential to model complex nonlinear dynamics [16]. The advanced modelling methods are inspired by the mindset of human brains or information transportation through neural cells, and not limited by good understanding of the mechanism of physical process [16]. The data-based modelling methods may be classified into two major categories by model logic, namely logic and neural networks (NN) based methods [16-19]. The former includes fuzzy algorithm, and support vector machine (SVM), Hammerstein and Wiener model, and fuzzy-

neuro algorithm. The latter includes artificial neural network (ANN), convolutional neural networks (CNN), radial basis function neural networks (RBFNN), multi-layer perception neural networks (MLPNN), extreme learning machine (ELM), and deep learning (DL). After trained by a large number of experimental datasets, the data-based modelling methods may achieve great predictive ability with less computational cost, compared with the traditional physical-based modelling methods. In addition, the data-based modelling is universally applicable to a large range of engineering problems, due to the little requirement of process mechanism, such as in civil engineering [20-22], environmental engineering [22, 23], medical engineering [24-27], energy and power engineering [28, 29], and computer engineering [30].

1.1.3 Bioaerosol and indoor air quality

Recently, indoor air quality (IAQ) receives much attention due to the effect on human health [31], as reported by the U.S Environmental Protection Agency [32]. According to previous studies in past two decades, indoor air was polluted more easily than the outdoor air by airborne particulate matter (PM), including dust, chemicals, and bioaerosols [33, 34]. The PM level should be controlled within a range especially in some specific buildings, such as hospitals, nursery schools, and laboratories [33, 35, 36]. Usually the indoor PM comes from various sources, for example, the human activities such as coughing and housekeeping, combustion of chemicals such as smoking and cooking, the physical behaviour of building materials such as emission and exfoliation, and organism propagation such as pollens and fungal spores. In addition, the concentration of indoor PM

may increase due to the poor air conditioning system without sufficient filtration, as well as the ventilation with the ambient air [31, 37, 38].

According to morphological characters of the diverse sources, PM in indoor air is classified into the two categories, namely bioaerosol and non-bioaerosol. The former is the aerosols that originate from organisms such as plants, microorganisms, and human beings, and suspend in the indoor air, attach or grow on the indoor surfaces [31, 37]. The bioaerosols consist of various compositions, including live or dead bacteria, viruses, fungi, pollens and their fragments and products [39]. Based on the experimental studies of long-term exposure to bioaerosols, bioaerosol is widely recognized as a hazard to public health. For example, it was reported by epidemiological investigations that some visible fungal existing indoor environment might increase the risk of infections, respiratory tract allergies, toxic effects and cancer to the residents, especially children and the elderly [39-43]. Human activities and air change between indoor and outdoor airs are the primary sources for the indoor bioaerosols [44]. On the other hand, the emission of fungi and spores from mouldy materials play another important role in the level of indoor bioaerosols [37].

Among all kinds of bioaerosols in the indoor environment, alive fungi and bacteria may be the most potentially harmful to human health, due to a relatively long time in the indoor environment. They also rapidly reproduce and release fungal spores if the environment is pleasant, such as temperature, humidity, and the nourished substrate. In addition, it was showed by experiments that structural faults on the inner building surfaces benefited to fungal growth [31]. In particular, indoor spaces are severely afflicted area to the issues such as basements, toilets,

warehouses, staircases, and kitchens. Furthermore, countries within the tropical marine climate, such as Malaysia and Singapore, may suffer from the issue, due to a comfortable environment for fungal growth with a small variational range of temperature and abundant rainfall [35, 45]. Therefore, control of the PM concentration at a healthy level should be considered seriously in the countries.

1.2 Motivation and objective

Based on the comprehensive literature review, several research gaps are figured out, as detailed below.

- As well known, it is extremely difficult to control two-phase flow due to complex two-phase flow and limited computational ability. Although a computational power is improved in last decade, simulation of multiphase flow still faces the challenge of trade-off between computational speed and accuracy. It was reported that over 8 million cells with 59 million-degree of freedoms were required for numerical simulation of pollutant dispersion process, and more than 40 minutes required for one main time loop with a four regions GPU (Graphics Processing Unit), and more than 8 hours with a four regions CPU (Central Processing Unit) [46]. It is almost impossible for traditional control algorithm to control a two-phase flow with an efficient computational speed.
- In addition, it is also very difficult to control the discrete-phase concentration in two-phase flow, due to the complex dynamics of the fluidic phase with the effect on the discrete phase. Most of the published studies focused on changing structure to achieve the control objectives of a desired steady two-phase flow. However, large numbers of simulation

and experimental work are required to obtain the optimized structure, and thus it is hardly realizable in a single-inlet fluid field with fixed geometric structure and working medium.

- Moreover, no study is published to implement a small variation of inlet flow to improve the local indoor air quality by reducing the bioaerosol concentration at an indoor corner. Although several experimental [2, 4, 16] and theoretical studies [25-27] were carried out for simulation and supervision of indoor PM, most of them only focused on the average concentration over global indoor space for the non-living particles initially suspending in the air. Apart from that, the air cleaners are always expensive with energy consumption due to long-term operation time, either working independently or within heat, air ventilation and cooling (HVAC) systems.

Therefore, regarding the above challenges, several objectives are achieved in this thesis, detailed as follows.

- Regarding the reduction of heavy computational cost, a data-based model may be a way to reproduce the dynamics of the two-phase flow, instead of solving physical-based mathematical equations, in order to reduce the complexity of the model. As such, it is more convenient for the controller design for two-phase flow.
- In terms of control of discrete-phase concentration in two-phase flow, probably the vortices in the two-phase flow are used as a medium that traps fluidic and discrete phase. With well-designed control algorithm on

the vortex, the optimization of discrete phase concentration may be achieved, via a small range of variation of the inlet flowrate.

- For improvement of local indoor air quality, the spores and fragments are controlled and then removed from the corners to prevent the accumulation of spores, by the advantage of the airflow from outlets of ventilation, air-conditioning systems, and other devices. On the other hand, the fungistat is brought into the corner area from the outlets of ventilation outlets or air conditioners. Then the fungistatic is conserved as much as possible, and mixed as long as possible at corners to prevent the spore growth. Taking into account the long operating time, the eco-friendly control methods are required with optimized energy consumption.

In order to meet these requirements, it is necessary to develop a two-phase model at a corner structure first for characterization of the flow pattern and particle motion discipline. The correlation between changes on inlet flow rate and particle concentration is further represented by a data-based model for convenience of controller design. The control algorithms are then designed and applied for obtaining an optimized discrete phase concentration. In addition, the optimization of energy consumption is also required for controller design strategies. Finally, the proposed methods are conducted to control the bioaerosol concentration at an indoor corner with optimized energy consumption, defined as the area around ceiling edges, in order to improve the indoor air quality which is very important to the resident health.

All in all, the thesis develops a data-driven based method for control of the discrete-phase concentration in a vortex-involved two-phase flow with optimized

energy consumption. The traditional CFD based flow model is replaced by different data-driven models, which contain the necessary characteristic information of the two-phase flow field, in order to improve the efficiency of controller design with optimized energy consumption in the proposed methods. In addition, the vortex is treated as an important medium for control of the discrete-phase distribution in a two-phase flow.

1.3 Thesis outline

This thesis is composed of six chapters, as graphically shown in Figure 1.2 and detailed below, and each chapter is further organized by several sections.

- Chapter 1 introduces the background of two-phase flow, machine learning techniques, and indoor bioaerosol pollutant issue, followed by the motivation, objectives, and scopes of the project.
- A comprehensive literature review is conducted systematically in Chapter 2, including the modelling of the two-phase flow, control strategies for two-phase flow, machine learning-based flow control, and biological dynamics of the indoor bioaerosols.
- Afterwards, Chapter 3 presents control strategy of particle concentration for two-phase potential corner flow with optimized energy consumption.
- Chapter 4 presents Neural Network-Model Predictive Control controller of particle concentration for control of two-phase laminar corner flow with optimized energy consumption.
- Chapter 5 presents a data-driven control of particle concentration within a turbulent corner flow via proportional-integral-derivative (PID) controller with optimized energy consumption.

- Finally, several conclusions are drawn based on preliminary work, and the future research works are proposed in the last chapter.

Figure 1.2 Thesis outline

Chapter 2 Literature review

This chapter presents a literature review for modelling methods of two-phase flow firstly in Section 2.1, followed by a review of the control strategies for two-phase flow in Section 2.2. The machine learning-based two-phase flow modelling and control are reviewed subsequently in Section 2.3. Finally, the literature review of the biological dynamics of indoor bioaerosols is conducted in Section 2.4.

2.1 Theoretical modelling of two-phase flow

For modelling of two-phase flow, the carrying medium is treated as continuous phase, based on the continuum assumption, for example, the gas phase in gas-particle two-phase flow, and the liquid phase in liquid-gas bubble flow. Except for the continuous phase, if the other phase accounts for small voluminal fraction of the two-phase flow with fixed shape, it is usually considered as discrete phase. In contrast, the other phase could also be treated as continuous phase for the large loading or voluminal fraction [8].

The literature review of theoretical modelling methods for two-phase flow are presented in this section. The modelling methods for continuous phase is reviewed through open literature in Section 2.1.1, followed by modelling methods for the discrete phase dynamics in Section 2.1.2. The literature review of modelling of the interaction between discrete and continuous phase is presented finally in Section 2.1.3.

2.1.1 Modelling of continuous phase dynamics

In terms of modelling continuous phase in two-phase flow, potential flow theory is one of the classic simplifications for complex fluid, by the assumption of inviscid and irrotational flows [47]. Based on the theory, a lot of studies were published for development of various point-vortex models with simplified flow consisting of several large-scale vortices, such as Rankine, Lamb-Oseen, Batchlor and Burge vortex models [48, 49]. For example, a potential point-vortex array model was applied by Kuwahara [50] for simulation of the two-dimensional vortex shedding phenome in the flow passing a cylinder, and for analysis of the relationship between the drag coefficient and attacking angle in the flow behind an inclined flat plate [51]. In addition, a discrete potential vortex model was developed by Sarpkaya and Schoaff [52] for determination of the vortex-street characteristics of an impulsively started flow around a circular cylinder, such as lift and drag forces, Strauhal number, oscillations of separation and stagnation points. Furthermore, the stream function was formulated for flow behind a bluff plane-based block, consisting of several point vortices and potential flow around the block, in which the interaction of the shear layers into steady vortex-shedding motion was amplified by a small disturbance [53].

Several studies were presented for incorporation of potential flow equation within a viscous flow for computational convenience [54, 55]. By the application of potential theory in a viscous flow, the degree of freedom was reduced from 10000 to 25 after proper orthogonal decomposition in the frequency domain by Epureanu *et al.* [54], with a good agreement against computational and experimental data. Furthermore, the interaction between potential flow and

viscous-wake was investigated for pressure disturbance propagation for the upstream blade rows in axial-turbine-blade rotor cascades [56].

Potential flow assumption is also applicable to model three-dimensional flow. For example, a potential flow model was used to analyse the unsteady flow through a three-dimensional industrial mixed-flow pump by van Esch *et al.* [57], in which the computational results had a great agreement with the experiments from global aspect. In addition, a three-dimensional incompressible potential airflow was assumed for the subsonic airflow around the shallow shell, to analyse the interaction of the vibration of the shell and the airflow [58].

Apart from that, laminar flow is effective for the analysis of flow characteristics for small Reynolds number, in which some exact or approximate solutions for NS equation may be achieved with simple geometries, such as steady flow between parallel plates, steady flow in a round tube, and steady flow between concentric rotating cylinders [1, 2]. For example, the wave formation was studied theoretically by Benjamin [59] through a uniform laminar stream for a viscous flow flowing down an inclined plane with a free outside surface at low Reynolds number, in order to analysis the mechanism of wave formation and estimate the formatted conditions and wave parameters. Moreover, the flow friction and pressure drop on highly curved helical pipes [60] and in a channel [61] were numerically simulated by laminar flow on CFD software, and validated by experiments from 3D-print model. Furthermore, simulations of a laminar flow passing over an inclined flat plate couple with thermal effects were studied by Yadav *et al.* [62] for the dust deposition, in order to address dust position problem for photovoltaic panel or a solar water heater. The three-dimensional flow in an

elliptical minicanal was simulated by Su *et al.* [63] in laminar flow with convective heat transfer to study the effects of Reynolds number and geometric structure on flow pattern. In addition, some other similar studies in laminar flow coupled with the heat transfer were reported by in different structures, such as flow in the interrupted microchannel heat sink with ribs in the transverse microchambers [64], non-circular ducts of a range of cross-sections [65], the entrance region of trapezoidal channels [66], square millimetric zigzag channels [67] and circular tubes [68].

On the other hand, for simulation of multiphase flow with turbulent effect on continuous phase, many works were published for CFD-conducted engineering process and theoretical analysis via several popular turbulent models, such as Reynolds-averaged Navier-Stokes (RANS), $k-\varepsilon$ model, large eddy simulation (LES) and direct numerical simulation (DNS). For example, the turbulent flow inside wall-bounded channel was numerically simulated by Haussmann *et al.* [69] at high Reynolds number through LES coupled with a lattice Boltzmann method, in order to predict the pressure drop of the flow. The direct material injection process of metallic powders from a nozzle was numerical analysis by a gas-solid model, in which the turbulent air was modelling by LES [70]. A gas-solid two-phase turbulent flow model was developed by Zhang [71] to analyze the separation of vortex sheet, subject to turbulence intensity and vorticity, in which higher collision probability of particles was observed by the increasing turbulent intensity and vorticity yield. The exergy loss in a duct was studied by the simulation of the liquid-solid nanofluid via a $k-\varepsilon$ method based turbulent regime with Reynolds number (5000 to 15000) [72]. A three-dimensional natural convection numerical model was conducted by Rath *et al.*

[73] for both laminar and turbulent flow on a stack of isothermal solid cylinders to investigate the influence of the numbers and arrangement of the cylinder to the airflow and thermal convection. The movement of the radioactive aerosols was simulated in a turbulent pipe flow to study the influence of the particle size and density on the transport and radioactive decay via DNS [74]. Numerical analysis for a turbulent cavitating flow around a wedge body was carried out by Kim *et al.* [75] to study the relationship between the shedding frequency of vortices and the development of cavitation, with satisfying validation result of wake flow characteristics against the experiments.

Furthermore, the fluid-solid flow at a wall-bounded region is one of the important two-phase flow problems, since the corner structure is very common in many applications, such as the design of disposable flow cytometers [76, 77] and fluid mixing problems [78]. Based on the fundamental investigation of the corner flow from published studies, when the fluid flowed along a corner, the blocking wall lead to backflow that forms a fluidic recirculation area with one or more vortices [78-80]. Experimental and theoretical studies on different corner flow dynamics were reported by Noack *et al.* [78] and Suh [80] based on different assumptions. For example, the stream function of the corner flow was modelled by mirrored-driven point vortices plus a stagnation flow as a quarter of the spin-up model with potential flow assumption [78, 80]. The stream function of a lid-driven corner flow was solved numerically by the matched eigenfunction method for a Stokes flow [81]. The similar crosswise velocity distribution pattern in the boundary layer was found by Rubin [3] between an incompressible corner flow and a quarter-infinite flat flow. The effect of the swept angle on flow pattern was experimentally studied for a compressible corner flow [82].

2.1.2 Modelling of discrete phase dynamics

As particles dispersing in the fluid, the dynamics of the particles is characterized by the force balance equation, namely Basset-Boussinesq-Oseen (BBO) equation, since the equation and its modified version are widely used for simulation of small particle movement at low Reynolds number, including the resistant, pressure gradient, added mass, Basset, Magnus, Saffman, buoyancy and gravity forces [83]. The resistance, also known as the drag force or frictional force, was firstly estimated for spherical objects with very small Reynolds numbers in a viscous fluid by Stokes in 1851 [8], after which a lot of researchers made a great effort to get high-precision theoretical and empirical formulas [84][52]. The pressure gradient force is caused by the pressure discrepancy around a particle that may be relatively large in a fluid field containing a vortex. Saffman and Magnus lift forces are caused by the particle rotation due to the velocity gradient on the particle or the post-collision to the wall [85].

The modification BBO equation was reported by a lot of published work for simulation of discrete-phase dynamics, by neglecting the small terms, and adding other forces if necessary, such as Brownian and Van der Waals forces. For example, the dynamics of bioaerosol with diameter smaller than $100\text{ }\mu\text{m}$ in office environment was simulated by Yu *et al.* [86] adding the Brownian force term and neglecting the Faxen term, based on the BBO equation. Wiener-diffusion term was added to BBO equation to simulate the solid-particle ($77\text{ }\mu\text{m}$) dynamics in a dilute gas-solid flow [87]. An extra thermophoretic term was employed by Zhuang *et al.* [88] to simulate the deposition of the airborne particles ($0.01\sim 10\text{ }\mu\text{m}$) in a room. Van der Waals force was added into the BBO

equation, since it was remarkable when a bioaerosol ($\leq 1 \mu m$) moved closely to wall at indoor corner, due to polarization among molecules [89]. The theoretical model, as well as the corresponding experimental studies, were investigated by Julien [53] for the dynamics of the fine sediment particles in a steady horizontal vortex, in which the very fine silts moved with a steady Rankine vortex, subjected to the pressure, centrifugal and frictional forces. Moreover, a combination of the drag force, gravitational force with the effect of buoyancy, Brownian force, Staffman force and thermophoretic force were taken into account for the simulation of particle dynamics inside an air-conditioning room [38], in which the model was validated by the simulation and experimental data conducted by Zhang *et al.* [54]. Apart from that, the collisions between wall and bioaerosols were also considered in the two-phase flow bounded by wall regions, according to the collision theory [9].

However, the above approach becomes impracticable due to the heavy computational resource requirement, if the millions of particles exist in the fluid, such as small particles mixing in chemical reaction processes. For the situation, the concept of “*particle cloud*” is proposed to represent the clustered properties of similar particles, in which three schemes are popularly used, namely Discrete Element Method (DEM), Discrete Parcel Method (DPM) and Eulerian modelling method [8].

2.1.3 Modelling of interaction between two phases

There are two well-known CFD schemes to model two-phase flow, namely the Eulerian-Lagrangian (E-L) and Eulerian-Eulerian (E-E) schemes. The E-L scheme is a classic one-way coupled modelling for two-phase flow, and widely

used for modelling of the interactions among the phases, with advantages in predicting turbulent diffusion with manageable computation [47-49]. Usually the fluid phase, or called carrier phase, is simulated via the Eulerian scheme, in which a control volume is defined, and the property of flowing fluid is expressed as a function of fields. However, the Lagrangian scheme is usually used to describe the interaction between the fluid and dispersed phases, which is tracked individually in the fluid field. The E-E scheme is generally used to describe many different types of multi-phase systems, in which all phases are formally treated as fluid, obeying the conventional fluid dynamical equations of motion [90].

Based on the published works on comparison between E-L and E-E schemes, both schemes showed good results with small error. A comparison of two schemes was conducted for gas-particle two-phase flow in a three-dimensional room by Zhao *et al.* [91], and for a two-phase flow over a backwards-facing step (BFS) by Tian *et al.* [90]. It was found that both schemes achieved satisfactory simulation results with comparison against experimental data [91, 92], however E-E was less computationally cost, while Lagrangian was marginally more accurate. Therefore, the choice of the two schemes generally depended on the computational ability, and simulation objectives of the model, as reported by Tian *et al.* [90]. It was necessary to choose E-L scheme, if the detailed trajectory of the individual particle is required. E-E scheme may be a good option, by contrast, due to the increasing computational cost by more particle number and longer simulation duration.

2.2 **Control strategies for two-phase flow**

The literature review of control strategies on two-phase flow problem are presented in this section. Control of two-phase flow may be generally classified into three categories, namely control by continuous phase fluid pattern in the subsection 2.2.1, control by structure design in the subsection 2.2.2, and control by reduced-order model in the last subsection.

2.2.1 **Control of continuous-phase pattern**

Control of two-phase flow may be achieved by control of continuous phase pattern, through prior understanding of the discipline of discrete phase movement driven by the carrier continuous phase. As presented by the open literatures, the spatio-temporal dynamic models for the continuous phase were developed via knowledge of the fluid field, in order to design the control algorithm by model-based control. For example, the interdisciplinary study of single-phase flow control was reported by Bewley [93] within wall-bounded domain, integrating science of control theory, fluid dynamics and computational methods. A standard linearized state-space model was converted by the nonlinear incompressible NS equation for the channel flow after Fourier transform for the control purpose. The optimal control was achieved to relaminarize a fully developed turbulent flow in a plane channel to minimize the influence of the turbulent energy and drag force via DNS [94]. It was further proved by Bewley and Aamo [95] that any other control approach at turbulent state failed to achieve sustained lower drag resistance than the laminar state in such channel flow. A feedback control aiming to increase the mixing effect was designed by boundary control laws for a 2D channel flow, starting from deviation of a Lyapunov-based approach based on NS equation [96]. A mathematical framework, involving the conditions of the

initial data and parameters, was established by Bewley and Temam [97] to guide the design of robust control in fluid mechanics, regardless of the disturbances from the numerical computation and measurements. Moreover, a feedback control strategy in boundary-layer flow system was theoretically proposed to maintain the laminar boundary layer via the linearized model based on boundary-layer approximation of NS equation, and verified by numerical simulations [98].

2.2.2 Control by structure design

Usually control strategy for two-phase flow by structure design is employed in a steady flow field, such as surrounding fluid in a percussion drilling process [99] and aerodynamic flow control of lift force on aircraft wings [100]. Several works were conducted on the strategy. As the most popular control strategy and proposed by Groth *et al.* in 1957 [101], the control laminar flow control (LFC) was used to maintain the laminar state to avoid the turbulent effects, Based on LFC, the wing geometry of an aircraft was designed by Joslin [102] via an inverse approach for a target pressure distribution through CFD, in which the control strategy for the suction flow rate was optimized by stability analysis of boundary-layer.

Other control strategy for two-phase flow were developed to address various issues. A jet with a coaxially compound structure was designed by Loscertales [103] to control the diameter of capsuled liquid aerosol via an electro-hydrodynamic actuator. Moreover, a microcapillary device was designed in a core-shell structure to optimize the shape of the produced double emulsion droplets in a two-emulsion flow [104]. The splitting of droplets in a T-junction was controlled by Link *et al.* [105] via parameter optimization of the structure

for two-emulsion flow. The dimension was studied as a critical parameter to process stability and reproducibility of two-phase diffusion in a fluid-fluid microchannel [106], and to the quality of bubbling process in a two-phase micro-flow-focusing (FF) [107]. Furthermore, the desired properties on thin liquid column sample stream was achieved by Huh *et al.* [77] via adjustment of channel geometry in an air-liquid two-phase microfluid system. Apart from that, improvement of the axial dispersion effects on particle size distribution was achieved by replacing microfluidic channels from a fluid-fluid two-phase flow to a gas-fluid-fluid three-phase flow [108].

2.2.3 **Controller design based on a reduced-order model**

Usually it is necessary to establish a reduced-order model to simplify the heavy computation work in two-phase flow simulation, such that the control design becomes practicable. According to the published works on fluid control by a reduced-order model, the detailed techniques could either be achieved by analytical linearization namely, white-box model [109], or direct system identification, namely black-box model [110]. A review of fluid flow control by linear system theory was published by Kim and Bewley [109], focusing on a feedback control implemented via placing actuators and sensors on the walls of the channel flow. In addition, non-linear dynamic models were also applied for flow control problems. For instance, an HW model was estimated by Karaca *et al.* [111] for vorticity control past a circular cylinder, in which a PID controller was then designed with good controlling performance. The vortices dynamics was translated to orbit model with lower order for the convince of the turbulence reduce control for a cross-flow plane [94]. The flow in a turbomachinery cascade was approximated by a reduced-order model in the frequency domain via proper

orthogonal decomposition (POD), to reduce the complexity of dynamic control [54]. Amplification of subcritical and supercritical instabilities was controlled by Debbagh *et al.* [112], via active closed-loop control in a 3D channel flow with magnetic effect, in which control laws were developed by a linearized discrete magneto-fluid coupled equations. The size of the droplets in was controlled by a proportional-integral (PI) controller to the inlet flow rate a T-junction microdroplet generator, based on the linear model of flowrate against droplet length, collected from the experimental measurements [113]. Apart from that, the widths of two-phase (liquid-liquid) steady mixing flows were controlled by the inlet flow rates of two phases, through a transfer function model derived by mathematical derivation in a Y-shaped microfluidic channel [114].

2.3 Machine learning-based modelling and control of two-phase flow

The recent development of control of fluid dynamics moves towards data-based black-box model or grey-box model as system identification techniques to obtain a reduced-order model. The review of open literature is conducted in detail for ML-based modelling and control methods of two-phase flow in this section. Starting with the review of ML implemented in fluid mechanics in Subsection 2.3.1, articles concerning the problem of ML applied in two-phase flow is reviewed subsequently in Section 2.3.2. Finally, the review of ML-based control methods is conducted in Section 2.3.3.

2.3.1 Machine-learning based fluid mechanics

With the blossom of the age of data in recent two decades, modelling of complex fluid dynamics was inspired by data-driven methods, e.g. neural networks,

especially the turbulence flow as a challenge for conventional fluid mechanics [115, 116]. Based on our best search and understanding, most of the published data-driven methods focus on the prediction of the fluid development, and seldom on the control of a multiphase flow problem. For example, Singh *et al.* [117] reconstructed the turbulent model by an NN for prediction of the lift and surface pressure on airfoils, in which the model discrepancies was trained as corrective forms for standard solver. The turbulent model in single-phase flow was developed effectively by Duraisamy *et al.* [115] via ML method to reduce uncertainties in turbulence, via the large and diverse data from experiments and direct numerical simulations. It was reported by Singh and Duraisamy [117] that the conventional Spalart-Allmaras model was reconstructed for turbulent flow over airfoils by NN through learning the discrepancy data from inverse problems, resulting in an improvement on prediction of lift force. The above method was also applied to model a turbulent boundary layer and bypass transition to turbulence, showing more rust and accurate than the tradition modelling methods [118]. The data-based NN was validated by Tracey *et al.* [119] with a great agreement to reproduce the results from the conventional CFD model for turbulent flow, without previously given the flow conditions. An ML model was simulated to predict dynamic flowing parameters with efficient computing efforts, such as CO₂ pressure, saturation and fraction, with different inlet scenarios for a CO₂ sequestration model in hydrocarbon reservoirs [120]. The parameters affecting the aerodynamic performance of a car was studied numerically by Uddin *et al.* [121] via NN based Monte-Carlo simulation, where the training data come from RANS based Realizable $k-\epsilon$ model by the CFD simulation. Furthermore, a liquid-particle flow was simulated for the drag-reducing particle

flowing within crude oil pipelines, via NN model, in which the results showed a great prediction accuracy [122].

According to open literature, computing speed and accuracy may be improved by ML techniques [118-120]. For example, the CNN based flow modelling methods computed much faster than GPU- and CPU-accelerated CFD solver on predicting a non-uniform steady laminar flow in both 2D and 3D domains [123]. In addition, a simplified cascade fuzzy NN model was trained to predict the critical mass flux and pressure in a critical flow, based on the fluid properties data from Henry-Fauske model, in which the prediction accuracies were much better than those in ordinary fuzzy neural network and support vector regression model [124]. Moreover, DL was used to reduce the model order in fluid simulation with much lower CPU cost and faster computational speed than the traditional CFD based simulation [125].

Apart from that, the performance of the conventional physical-based turbulent model may be improved incorporating with ML methods, by predicting the nonlinearity that is difficult for conventional methods. For example, based on the review of open literature, although RANS equations were widely used in turbulent modelling, it was still lack of universally predictive capabilities, resulting in limitations on predictive accuracy [126, 127]. The mean flow feature was trained by the data generated via DNS, to predict Reynolds stress discrepancies by RANS equations, in turbulent flows in a square duct and massive separation flow [127]. The ML was proposed by Wu *et al.* [126] to predict linear and nonlinear blocks in Reynolds stress tensor in RANS turbulent model separately, to augment the prediction ability for an ill-conditioned problem.

A DL-NN architecture was reported by Ling *et al.* [128], to improve the prediction accuracy of anisotropy tensor in RANS model.

Regarding the control strategy for fluid based on the learning process, the basic concept was reviewed by Fu [129], in which the optimal control methods was incorporated with the learning algorithm for the system lacking prior knowledge. The inefficient information was learnt or estimated by the controller in the plant system, with more and more input and output data imported into the controller [129]. For example, an interactive learning control approach was proposed by Chen *et al.* [130] to obtain the desired laminar flow position in the similar Y-shaped two-fluid mixing channel based on the experimental trials, regardless of a flow model [130]. However, timely updating of the control algorithm and repetitive operations were required by this control strategy, resulting in high commutating cost. Moreover, it was necessary to make extra efforts on improving the control accuracy, especially in the beginning of the process and on solving the problems, such as control of a nonstationary system, improvement of the learning rate, construction of the stop rule, and development of hierarchical structure [129].

ML algorithms might be also used in data-based system identification for control purpose and design of sensor placement [18]. For example, an ML-based closed-loop separation control was experimentally developed by Gautier *et al.* [131] on a backwards-facing step flow at $Re=1350$ to reduce the recirculation zone, in which the control law was generated based on a genetic learning programming via the feedback data from an optical sensor. The dynamic behaviour was identified by NN for the prediction of wall-shear stress due to wall

actuation, in which an adaptive inverse model control was further designed for drag reduction [132]. Furthermore, the Coriolis mass flowmeter was improved by Yue *et al.* [133] to real-time measurement of gas-liquid flow, by Support Vector Machine algorithm inserted in DSP and FPGA to correct the real-time error online.

2.3.2 Machine-learning based two-phase flow

Although a lot of published studies were conducted on implementing the data-based methods for single-phase fluid modelling [18] as presented in Section 2.3.1, only a few articles were reported for two-phase flow modelling and control problems. The studies on ML-based two-phase flow control were more like independent researches based on problem-driven issue, instead of a systematically thermotical analysis on two-phase flow control via machine learning techniques. For example, the link between two-fluid dynamics and so-called “closure terms” was established by Buist *et al.* [134] via NN, performing better predictive ability than the conventional methods. The void fraction was estimated by a well-trained NN for gas-liquid flow in a Venturi tube, via the data experimentally collected by two differential pressure signals, with good predictive accuracy for high the mixture velocity [135]. An SVM based image processing techniques were implemented by Zhou *et al.* [136] to excellently classify the different flowing regimes within a short process time, for the two-phase flow in a horizontal tube, with the image experimentally collected by digital high-speed video.

2.3.3 Machine-learning based control methods

Among all the controller design algorithms proposed based on ML model, model predictive control is one of the most popular algorithms for engineering process, due to good adaptation on nonlinear dynamics model [137]. The design of MPC based on NN was formulated and valid by Ławryńczuk [133, 135, 136] and Janakiraman *et al.* [134] via the simulations of different processes, in which NN is linearized by Taylor approximation and MPC then developed by solving a quadratic optimization problem. The proposed MPC-NN controller presented good control performance [138]. In addition, MPC was also implemented to control nonlinear dynamics in distillation column system based on a two NN combination model, presenting high control accuracy with good efficiency, in which one NN processes the history information and the other one estimates the time-variant response [139]. Furthermore, MPC was designed by Ławryńczuk [140] for a multivariable process based on Wiener-NN model, in which Wiener block captured the linear dynamics and NN the steady-state nonlinear dynamics of the plant. Another MPC controller was developed based on a linearized ELM model for a homogeneous charge compression ignition engines, in which ELM was trained by experimental data capturing the engine dynamic behaviour [141, 142]. Apart from that, a nonlinear MPC by Santos *et al.* [143] was proposed to optimize the humidity during the drying process of medium density fiberboard, based on data-based grey-box model, in which the speed of setpoint tracing was significantly improved, comparing to the conventional single-input-single-output PID controller.

Other various ML-based control strategies in published literature are exemplified below. A new effective control strategy, namely optimal bipartite

consensus control, was developed by Peng *et al.* [144] via NN that described the cooperative and competitive dynamics among unknown agents in the systems. Real-time traffic information was refined by Garg *et al.* [145] via a vision-based deep reinforcement learning to enhance the traffic light control system at road intersections. Moreover, a PID controller tuned by Ziegler and Nichols methods, was compared to another controller designed by genetic algorithm-based adaptive neuro-fuzzy inference system (GANFIS), for control of a nonlinear DC motor, in which the ANFIS based GA had much better performance on response speed, rise time and settling time by simulations [146]. In addition, a fuzzy NN controller was developed by Fung *et al.* [17] to replace the traditional mathematical kinematic model for control of motor quick-return with experimental validation.

Remarkable performance is presented by NN-based control. For example, NN was implemented to inverse kinematic control of robot joint angles, replacing the traditional Jacobian matrix based control, to avoid the inaccurate parameters and invertible matrix [147, 148]. NN-based inverse dynamics controllers were designed by different learning architectures for robot dynamics control, such as generalized [149], specialized architecture [150], and hybrid learning architectures [151]. Two NNs were incorporated to determine the robot hand movement as parts of learning control system, detailed by one NN learning to generate command signals by sensor outputs, and the other learning the relationship between changes in command signals and sensor outputs [152, 153].

2.4 Indoor bioaerosols dynamics

One of the applications for control of two-phase corner flow is the local bioaerosol concentration management at an indoor corner by the airflow from the ventilation outlet located at the ceiling. The literature review of indoor bioaerosols dynamics is conducted in this section. The modelling and experimental works of indoor bioaerosol dynamics are reviewed firstly in Section 2.4.1, followed by the impact on growth and release of indoor bioaerosol in Section 2.4.2. Finally, the review of the impact on bioaerosol dynamics is reported in Section 2.4.3.

2.4.1 Modelling and experiment of indoor bioaerosol dynamics

Based on the published experimental and theoretical studies, it was more easily for microorganism to grow, propagate and release bioaerosols at indoor corner due to the suitable environment, such as low flow rate, proper humidity and temperature [31, 37, 38, 154]. For example, a higher concentration of indoor particle matters was found experimentally by Li *et al.* [155] at indoor corners with natural ventilation. Moreover, the changed geometry and material of the building envelope generate thermal bridges to increase the local heat flux density and then to change internal surface temperature. The decrease in surface temperature leads to condensation, which was helpful for mold growth. On the contrary, the increasing local temperature generated the stagnation air to promote mold growth [128-131]. Other effects, such as the coarse surface of the corners and organic content on the building material surfaces, also played important roles in promoting the germination and mold growth on the wall surfaces. In addition, the increase of air velocity might contribute to releasing spores and fragments

from the mold [124, 132, 133]. Furthermore, usually it was inconvenient to clean the upper corners, which was additional benefit of the mold growth.

In general, the spores and fragments disperse into the room with the carrier airflow after released from the hyphae. The dynamics of the bioaerosols was influenced by their size, evolution due to the changeable environment, and the carrier flow pattern with the dominant effect [126]. Among the three effects, only the carrier flow pattern may be controlled to tune the particle behaviors via a moving vortex, such that the desired residual particle concentration is achieved.

2.4.2 Impact on growth and release of indoor bioaerosols

Several previous studies show that some environmental effects, such as the airflow rate, temperature, relative humidity and building materials, play an important role in the growth, propagation, and spread of the bioaerosols at indoor corners. They are detailed below.

2.4.2.1 Airflow rate

Experimental studies published reveal the relationship between the air velocity and the release of fungal spore and fragments. For example, it is shown that the increase in airflow rate enlarges the release of both fragments and spores [154], in which fragments are released more than the spores. In other words, more particles with larger size are released into the corner with increasing the air velocity. A similar conclusion was also found experimentally for the fungi *Botrytis cinerea* [156], in which airflow enables *Botrytis cinerea* to aerosolize conidia and fragments. The variations of the airflow velocity with both the quantity and diameter of the released spores were studied experimentally for two

kinds of fungi, *Penicillium chrysogenum* and *Trichoderma reesei* [157], in which higher air velocities enhance the quantities of the released particles for both the fungi, and *Penicillium chrysogenum* tends to release more particles with larger size, while *Trichoderma reesei* works on the contrary.

2.4.2.2 Temperature

The microbial volatile organic compounds were tested via *Aspergillus flavus* as a kind of fungi that could produce dangerous secondary metabolites in a laboratory environment [158], in which *Aspergillus flavus* tended to produce most metabolites at 30-degree Centigrade.

2.4.2.3 Relative humidity

It is essential for water to aerosolize bioaerosols. By the experimental work of fungi called *Botrytis cinerea* [156], it was demonstrated that the relative humidity had a remarkable effect on the size of the aerosolized particle, in which smaller size of particles was released easily with lower relative humidity. The similar experimental results were also observed [159], in which the quantities of secondary metabolites increased with the decrease of the humidity. Besides, it was observed experimentally [160] that more particles were released at low RH (< 42%) than those at high RH (> 70%) for both *Aspergillus fumigatus* and *Penicillium*.

2.4.2.4 Building materials

Many relevant experimental works were carried out for analysis of the influence of fungi on different building materials. For example, regarding the metal materials in the HVAC system, the copper tended to have a better

performance than the aluminium in preventing the material from erosion caused by the bioaerosols in the same environmental conditions [161]. However, for the wooden-related materials, it was shown by several experiments [159] that wooden-related materials were a more suitable substrate for mould growth, compared with gypsum and ceramic materials.

2.4.3 **Impact on bioaerosol dynamics in airflow**

Several previous studies showed that, after the bioaerosol released from the substrate, its dynamics in the airflow is influenced by several effects, such as particle size, the airflow pattern, and the evolution of the particles, which are detailed below.

- Particle size It was shown by both experiments and simulations that particles with different sizes moved along different trajectories in the airflow [37, 38, 162]. The size of indoor PM ranges largely, and thus the indoor PM is generally classified into three categories due to their diameters, namely the ultrafine, accumulation and coarse [37]. The smaller particles follow airstream closely, while the behaviour of larger particles is strongly influenced by their mass due to the larger inertia [37]. By computational fluid dynamics (CFD) simulations of the transport of indoor particles [162], it was shown that smaller particles tended to follow the airflow and to move with the airflow onwards, while larger ones fallen down onto the floor after a period of time.
- Airflow pattern The airflow pattern is one of the key effects of driving the bioaerosols after released from the substrate. For example, it was shown by numerical simulations [38] that the movement of the particles was

significantly different between central- and split-type air-conditioning rooms, in which the different positions of air-conditioners resulted in different airflow patterns.

- Evolution of the particles Usually the particles such as pollens experiences a change in geometrical shape when the external environment varies. A shape-folding pattern of pollen was investigated when it was exposed to the dry environment, resulting in a decrease of cellular volume, while the shape would get recovered once the pollen was exposed to a humid environment [163]. This volumetric variation affects the pollen dynamics in the air if the environment varies.

However, no published study has been found on the control of indoor bioaerosol concentration at corner via benefitting from the airflow from the ventilation outlet with long-term effectiveness with optimized energy efficiency.

2.5 **Remarks**

In summary, the previous published theoretical and simulation works focus on the modelling of the two-phase flow dynamics upon physical and mathematical views, through getting a better cognition of the physical process to improve physical-based model, making assumption to simplify the flow model, or improving computational power to achieve numerical solutions. In addition, the previous published data-based modelling works concentrate on reproducing the dynamics of single-phase flow, or improving the accuracy of existing flow model as an auxiliary term. However, how to achieve a desired discrete-phase

concentration in an energy-efficient way has not been involved. As such, several remarkable ideas proposed from the present work are described below.

- A two-phase corner flow with fix geometry is considered in present work, in which the inlet flowrate is the only approach to modulate the flow pattern;
- In the above flow domain, two-phase corner flow models involving a recirculation zone are developed to trace the particle dynamics, based on different continuous-phase assumption or flow state, such as potential flow, laminar regime and turbulent regime, respectively.
- The relationship between the inlet flow rate and the residual particle concentration is then studied by different data-based methods, including orthogonal experiment design methods, NN, and system identification via linear transfer function model;
- Based on the above data-based models, the optimized control strategies are studied to achieve a desired residual particle concentration, including orthogonal design, MPC and PID control strategies.
- Energy consumption on control activity is optimized as an essential part of the control algorithm, with an adjustable weight factor balancing the consumed energy and control effectiveness.
- The proposed control strategies are conducted to improve the local indoor air quality by reducing the bioaerosol concentration at an indoor corner, defined as the area around ceiling edges.

The development of the gas-particle two-phase flow model in different schemes, as well as design corresponding control strategies for control of discrete phase concentration, are presented in the following chapters, respectively.

Chapter 3 Development of control strategy of particle concentration for two-phase potential corner flow with optimized energy consumption

In this chapter, a feasibility study based on airflow-controlled approach is proposed to control the bioaerosol concentration at an indoor corner with optimized energy consumption, based on the two-phase potential corner flow model with the chaotic moving vortex. The two-phase potential flow model is developed first to characterize the flow pattern and airborne particle dynamics at the indoor corner via E-L method. Based on the model, continuously released particles are simulated to indicate the probability of bioaerosol movement, which is released sparsely and randomly by microorganisms at corner in a real situation, since their growth and aerosolization are difficultly predicted and detected [164, 165]. Therefore, control of the residual particle concentration is motivated to reduce or increase the particles remained at the indoor corner, instead of control towards a low number of particle movements. A controlling process is thus required to be open-loop, sustainable, repeatable, energy efficient and easily implementable. The open-loop control strategies are then developed to optimize bioaerosol concentration through energy consumption by an orthogonal scheme with two kinds of commonly used control input signals, namely Heaviside Step Function (HSF) and Pulse Width Modulation (PWM). The desired control objectives depend on different scenarios, for example, to minimize the local bioaerosol concentration with optimized energy consumption, when the bioaerosols are released from the sources around the corner with a constant speed. In terms of the detergent released from the ventilation outlet, however, it is

expected for the control activity to maximize the local bioaerosol concentration with optimized energy consumption. Finally, several guidelines of control strategies are proposed practically to improve the local indoor air quality with efficient energy consumption.

The problem is stated firstly in Section 3.1. After that, the theoretical derivation of two-phase potential corner flow model is presented in Section 3.2, including modeling of flow pattern and particle dynamics. The two-phase flow model is validated against published experimental and simulation results, as shown in Section 3.3. The simulation configuration and results are discussed in Section 3.4, subject to five case studies. Finally, the remarks of the proposed methodology are presented in Section 3.5.

3.1 Problem statement

Figure 3.1 Schematic of the indoor corner with pollution of bioaerosols

The indoor corner in presented work is defined as the area around the edges of the ceiling. The schematic illustration of the indoor corner is shown in Figure 3.1. Usually, people install the ventilation outlet only for pumping the fresh or

conditioned air into a room. Nevertheless, the airflow from the ventilation outlet is also feasible to remove the released bioaerosols at the corner or carry detergent to avoid bioaerosol growth according to presented work. Most of the real indoor corners have an infinite length on the horizontal direction, represented by z -axis, such that they may be simplified as a 2D right angle. As shown in Figure 3.2, a right angle with two semi-infinite sides is defined as the computational domain for potential corner flow, in which a specific square zone at the corner is called as *the corner zone* for evaluation of the residual particle concentration, and the air is exhausted from the ventilation outlet into the corner zone along the vertical edge. Apart from that, the particles are released either from the wall, as shown in Figure 3.2(a), or from the ventilation outlet, as shown in Figure 3.2(b), based on the different requirements, and then they move with the carried airflow. Here, particles are released with a fixed time interval to indicate the probability of rarely released ones. For example, they may be removed out of the corner zone with higher probability in a real situation, if the residual particle concentration is reduced in the corner zone during simulations. A short distance is set up initially between particles and wall, represented by d_p in Figure 3.2(a), in order to simulate the substrate of microorganisms. Theoretically, several assumptions are made as follows: (1) incompressible and potential is considered inside the corner; (2) no collision is considered among particles due to the low density; and (3) there is no influence on airflow due to particle movement due to the small particle size.

Figure 3.2 Schematics of corner flow with bioaerosols, (a) bioaerosols released from partial ceiling and wall, (b) bioaerosols or detergents released from ventilation outlet

3.2 Modeling of two-phase potential corner flow

In this section, the flow pattern at the corner is formulated via potential flow theory which contains a stagnation flow and a moving vortex [78, 80]. The velocity of the mixture fluid field is given in Section 3.2.1, and the trajectory of the point vortex is investigated subsequently.

3.2.1 Flow pattern at corner

3.2.1.1 Velocity field of the potential corner flow

Potential flow area

According to the published paper, a corner flow may be considered as a part of spin-up model, which is further expressed in a form of potential flow with a stagnation flow plus a point vortex, in which the stagnation flow is driven by the external flow generated by the ventilation outlet with an initial intensity k . The vortex in the corner flow moves in the anti-clockwise

direction due to the increasing separation flow generated at the upstream wall [80]. Therefore, the potential streamline function Ψ_{oc} is given by

$$\Psi_{oc} = \Psi_s + \Psi_c + \sum_{n=1}^4 \Psi_{nv} \quad (3.1)$$

where $\Psi_s = k_s xy$ is the streamline for original stagnation flow. $\Psi_c = e(t)xy$ is the streamline for controlled flow [166], where the intensity of control input $e(t)$ is associated with the accumulated energy consumption $E(t)$ via $e(t) = \sqrt{dE(t)/dt}$. Ψ_{nv} are the streamlines for the Rankine point vortices with a vortex core radius r_0 , given by

$$\Psi_{nv} = \begin{cases} -\frac{\Gamma}{2\pi} \ln |\mathbf{P} - \mathbf{P}_n|, & |\mathbf{P} - \mathbf{P}_n| \geq r_0 \\ -\frac{\Gamma}{4\pi r_0^2} |\mathbf{P} - \mathbf{P}_n|^2 & |\mathbf{P} - \mathbf{P}_n| < r_0 \end{cases} \quad (3.2)$$

where Γ is the circulation of the vortices and $\Gamma > 0$ when the vortex moves in an anti-clockwise direction, and $\mathbf{P} = (x, y)$ the interested position. The whole flow field at the corner is induced by one vortex located $\mathbf{P}_1 = (x_1, y_1) = (x_v, y_v)$ in the first quadrant, and the other three virtually mirrored vortices located at $\mathbf{P}_2 = (x_2, y_2) = (-x_v, y_v)$, $\mathbf{P}_3 = (x_3, y_3) = (-x_v, -y_v)$, and $\mathbf{P}_4 = (x_4, y_4) = (x_v, -y_v)$, respectively. The velocity field $\mathbf{u} = (u_x, u_y)$ if $|\mathbf{P} - \mathbf{P}_1| \geq r_0$ is given by

$$\begin{cases} u_x = \frac{\partial \Psi}{\partial y} = k_s x + e(t)x + \sum_{n=1}^4 \frac{(-1)^n \Gamma}{2\pi} \frac{y - y_n}{|\mathbf{P} - \mathbf{P}_n|^2} \\ u_y = -\frac{\partial \Psi}{\partial x} = -k_s y - e(t)y - \sum_{n=1}^4 \frac{(-1)^n \Gamma}{2\pi} \frac{x - x_n}{|\mathbf{P} - \mathbf{P}_n|^2} \end{cases} \quad (3.3)$$

The velocity field $\mathbf{u} = (u_x, u_y)$ within the vortex core area is obtained by solving Navier-Stokes(NS) Equation (3.4) with the boundary conditions for velocity $\mathbf{u}_c = (u_{cx}, u_{cy})$ and pressure gradient $\nabla p_c \cdot \mathbf{u}_c$ is given by substituting $|\mathbf{P} - \mathbf{P}_1| = r_0$ into Equation (3.3). The pressure gradient at the boundary of the vortex core ∇p_c is solved by 2-D NS equation at $|\mathbf{P} - \mathbf{P}_1| = r_0$.

$$-\frac{1}{\rho_f} \nabla p = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \quad (3.4)$$

where ρ_f is the fluid density, ∇p the pressure gradient and $\nabla = (\partial/\partial x, \partial/\partial y)$ the Hamilton operator. It is obvious that Equation (3.5) is a theoretical solution for the condition $|\mathbf{P} - \mathbf{P}_1| < r_0$ that satisfies with the boundary conditions $\mathbf{u}_c$ and ∇p_c , given by

$$\begin{cases} u_x = k_s x + e(t)x - \frac{\Gamma(y - y_1)}{2\pi r_0^2} + \sum_{n=2}^4 \frac{(-1)^n \Gamma}{2\pi} \frac{y - y_n}{|\mathbf{P} - \mathbf{P}_n|^2} \\ u_y = -k_s y - e(t)y + \frac{\Gamma(x - x_1)}{2\pi r_0^2} - \sum_{n=1}^4 \frac{(-1)^n \Gamma}{2\pi} \frac{x - x_n}{|\mathbf{P} - \mathbf{P}_n|^2} \end{cases} \quad (3.5)$$

Boundary layer area

In the fluid boundary layer, viscosity force is larger than the inertia in general, leading to a large velocity gradient, which often results in turbulence and makes fluid computation much more difficult and complicated. In the presented model,

the boundary layer is defined as a thin layer on both ceiling and wall. The velocity at the outmost boundary is computed by submitting $x = 0$ into Equation (3.3) for the boundary layer on y axis, and $y = 0$ for boundary layer on x axis. As well known, many techniques based on NS equation are developed for solution of the velocity field in the boundary layer. One of them is the Blasius similarity solution theory for time-independent flow and it is used here to approximate the velocity u_b and pressure fields p_b in the boundary layer, given by [167]

$$u_{bx} = Uf'(\eta), \quad u_{by} = \frac{1}{2}\sqrt{\frac{\nu U}{x}}[\eta f'(\eta) - f(\eta)] \quad (3.6)$$

$$\frac{\partial p_b}{\partial x} = -\rho\left(\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x}\right) \quad (3.7)$$

where U is the potential velocity outside of the boundary layer, ν the kinematic viscosity of the fluid, $\eta = y\sqrt{U/\nu x}$, and $f(\eta)$ is numerically solved by Howarth [89], and the momentum boundary layer thickness is computed by

$$\theta = 0.664\sqrt{\frac{\nu x}{U}} \quad (3.8)$$

It is noted that the potential velocity U outside of the boundary layer by Equation (3.3) is a function of time and spatial variables. However, the variation of U with time and spatial variables is small and neglectable in current case, such that the similarity theory on the presented model is reasonably used for an approximate solution on the boundary layer.

3.2.1.2 Trajectory of the point vortex

The vortex in Quadrant 1 is induced by the other three mirrored vortices in Quadrants 2, 3, and 4 due to the no-penetration condition at the walls, as well as the original stagnation flow and controlled flow. If the vortices located at Quadrants 2, 3 and 4 are considered only, the streamline Ψ_t of these vortices is expressed as

$$\Psi_t = k_s xy + e(t)xy + \sum_{n=2}^4 \frac{(-1)^n \Gamma}{2\pi} \ln |\mathbf{P} - \mathbf{P}_{nv}| \quad (3.9)$$

Based on the potential flow theory [1], after substituting the target location $\mathbf{P}_v = (x_v, y_v)$, where $y_v > 0$, into Equation (3.3), we have

$$\begin{cases} u_{vx}|_{x=x_v, y=y_v} = k_s x_v + e(t)x - \frac{\Gamma}{4\pi} \frac{y_v}{x_v^2 + y_v^2} + \frac{\Gamma}{4\pi} \frac{1}{y_v} \\ u_{vy}|_{x=x_v, y=y_v} = -k_s y_v - e(t)y - \frac{\Gamma}{4\pi} \frac{1}{x_v} + \frac{\Gamma}{4\pi} \frac{x_v}{x_v^2 + y_v^2} \end{cases} \quad (3.10)$$

3.2.2 Particle dynamics

Potential flow area

The motion of a particle is determined by the net force in the flow field. The force analysis is conducted in potential flow area first, and then in the boundary layer area. In potential flow area, the particles inside the fluid field are mainly subjected to four kinds of force, the pressure force $\mathbf{F}_p$ caused by the gradient of pressure due to the ununiform pressure field generated by the moving vortex, friction $\mathbf{F}_f$ caused by relative velocity, gravity $\mathbf{F}_g$ and buoyancy $\mathbf{F}_b$. Other forces are neglected since the velocity gradient is not

very large in potential flow area. The net force $\mathbf{F}_{\text{pfa}}$ for a particle is thus expressed as [9]

$$\mathbf{F}_{\text{pfa}} = \mathbf{F}_p + \mathbf{F}_f + \mathbf{F}_g + \mathbf{F}_b = -\frac{\pi d_p^3}{6} \nabla p + 3\pi d_p \nu \rho_f \mathbf{u}_r + \rho_p \mathbf{g} \frac{\pi d_p^3}{6} - \rho_f \mathbf{g} \frac{\pi d_p^3}{6} \quad (3.11)$$

where d_p is the particle diameter, ρ_p the particle density, $\mathbf{u}_r = \mathbf{u} - \mathbf{u}_p$ the relative velocity of the two phases, $\hat{\mathbf{u}}_r$ the unit vector of $\mathbf{u}_r$, and $\mathbf{g}$ the gravity acceleration.

Boundary layer area

On the other hand, other forces in the boundary layer area, such as Saffman lift force, Magnus force, and Van de Waals force, may not be neglected due to the large velocity gradient if particles are close to wall or ceiling. Therefore, the resultant force is expressed as

$$\mathbf{F}_{\text{bla}} = \mathbf{F}_p + \mathbf{F}_f + \mathbf{F}_g + \mathbf{F}_b + \mathbf{F}_{\text{sl}} + \mathbf{F}_m + \mathbf{F}_{\text{LvdW}} \quad (3.12)$$

where $\mathbf{F}_{\text{sl}}$, $\mathbf{F}_m$ and $\mathbf{F}_{\text{LvdW}}$ represent Saffman lift force, Magnus force and Van de Waals force, respectively.

Saffman lift force is caused by the particle rotation due to the velocity gradient on the particle or the post-collision to the wall. Mei [85] proposed an empirical equation to evaluate the lift force at Reynolds number less than 40, given by

$$\begin{aligned} \mathbf{F}_{sl} = & 1.61d_p^2\rho_f\sqrt{v}\left|\nabla\times\mathbf{u}_r\right|^{-\frac{1}{2}}\left[\mathbf{u}_r\times(\nabla\times\mathbf{u})\right]\left[(1-0.3314\beta^{1/2})\exp\left(-\frac{d_p\left|\mathbf{u}_r\right|}{10v}\right)\right. \\ & \left.+0.3314\beta^{1/2}\right] \end{aligned} \quad (3.13)$$

where $\beta = (d_p/2|\mathbf{u}_r|)|\nabla\times\mathbf{u}|$ and $\nabla\times\bullet$ represents the curl of a vector.

Magnus force is another lift force developed due to the particle rotation, and expressed by

$$\mathbf{F}_m = \frac{\pi}{8}d_p^3\rho_c\left[\left(\frac{1}{2}\nabla\times\mathbf{u}-\omega_d\right)\times\mathbf{u}_r\right] \quad (3.14)$$

where ω_d is the angular velocity of the particle.

In addition, particles are influenced by London-Van der Waals(LvdW) $\mathbf{F}_{LvdW}$ to remain attached on the wall, when they are transported close to the wall surfaces by airflow, due to either initially particle releasing or resuspending after collision from the wall surfaces. $\mathbf{F}_{LvdW}$ may be approximately formulated by neglecting the repulsive effect through Lifschitz approach, if the dispersion between the molecules is dominated [168], given as

$$\mathbf{F}_{LvdW} = \frac{hvd_p}{16\pi d^2} \quad (3.15)$$

where d is the vertical distance between particle and wall surface, h the Planck's constant, and ν the frequency. $E_L = h\nu$ ranges from 0.6 to 9.0 eV by different material properties [169].

Apart from that, Brownian motion of a particle is considered in the boundary layer, since both flow and particle velocities are relatively small. Brownian motion is thus expressed as

$$|\bar{X}|^2 = \frac{2K_B T}{3\pi\nu} \frac{2t_h}{d_p} \quad (3.16)$$

where $\bar{X}$ is the root mean square particle displacement, K_B the Boltzmann constant, T the temperature, and t_h the holding time.

In addition, a flat wall and inelastic particles are considered during the collision, and the velocities of a particle between pre-and post-collisions are formulated below with the two conditions,

$$\text{if } \frac{u_y^{(0)}}{|\mathbf{u}|} < -\frac{2}{7f(1+e)}, \text{ then } u_x = \frac{5}{7}(u_x^{(0)} - \frac{d_p}{5}\omega_d^{(0)}); u_y = -eu_y^{(0)}; \omega_d = -\frac{2u_x}{d_p} \quad (3.17)$$

$$\text{if } -\frac{2}{7f(1+e)} < \frac{u_y^{(0)}}{|\mathbf{u}|} < 0, \text{ then}$$

$$u_x = u_x^{(0)} + f(1+e)u_y^{(0)}; u_y = -eu_y^{(0)}; \omega_d = \omega_d^{(0)} + \frac{5}{d_p}f(1+e)u_y^{(0)} \quad (3.18)$$

where f and e are the coefficients of friction the restitution, and velocities with superscript (0) indicate those before the collision [8].

In order to evaluate the particle movement, the residual particle concentration C_{ip} at time τ_i is defined as

$$C_{ip} = \frac{1}{t_s - t} \int_t^{t_s} \frac{N_{ip}}{A} dt \quad (3.19)$$

where N_{ip} is the number of particles inside the corner zone at time t , $t_s - t$ the smooth duration and A the area of the corner.

3.2.3 Nondimensionalization and numerical flowchart

For parameterization of the modeling, the non-dimensional parameters are defined as follows,

$$\tau = \frac{t}{t^*}, \quad \bar{P} = \frac{P}{l^*}, \quad \bar{u} = \frac{u}{v^*}, \quad \bar{F} = \frac{F}{F^*} \quad (3.20)$$

where $t^* = 1/k_s$, $l^* = \sqrt{-\Gamma/2\pi k_s}$ ($\Gamma < 0$), $v^* = \sqrt{\frac{-\Gamma k_s}{2\pi}}$, and $F^* = l^* M_p / t^{*2}$ ($M_p = \pi \rho_p d_p^3 / 6$ indicates the mass of a single particle) represent the characteristic time, length, velocity and force respectively.

Based on Equations (3.3), (3.5) and (3.6), the fluid velocities $\bar{u}$ are nondimensionalized as

Potential flow area

$$\begin{aligned}
& \text{if } |\bar{\mathbf{P}} - \bar{\mathbf{P}}_1| \geq \bar{r}_0 \\
& \bar{u}_x = [1 + \bar{e}(\tau)]\bar{x} + \sum_{n=1}^4 \frac{(-1)^n (\bar{y} - \bar{y}_n)}{|\bar{\mathbf{P}} - \bar{\mathbf{P}}_n|^2} \quad \bar{u}_y = -[1 + \bar{e}(\tau)]\bar{y} - \sum_{n=1}^4 \frac{(-1)^n (\bar{x} - \bar{x}_n)}{|\bar{\mathbf{P}} - \bar{\mathbf{P}}_n|^2} \\
& \text{if } |\bar{\mathbf{P}} - \bar{\mathbf{P}}_1| < \bar{r}_0 \\
& \bar{u}_x = [1 + \bar{e}(\tau)]\bar{x} + \frac{\bar{y} - \bar{y}_1}{\bar{r}_0^2} - \sum_{n=2}^4 \frac{(-1)^n (\bar{y} - \bar{y}_n)}{|\bar{\mathbf{P}} - \bar{\mathbf{P}}_n|^2} \\
& \bar{u}_y = -[1 + \bar{e}(\tau)]\bar{y} - \frac{\bar{x} - \bar{x}_1}{\bar{r}_0^2} + \sum_{n=2}^4 \frac{(-1)^n (\bar{x} - \bar{x}_n)}{|\bar{\mathbf{P}} - \bar{\mathbf{P}}_n|^2}
\end{aligned} \tag{3.21}$$

Boundary layer area

$$\bar{u}_{bx} = \bar{U}f'(\bar{\eta}) \quad \bar{u}_{by} = \frac{1}{2}C_b \sqrt{\frac{\bar{U}}{\bar{x}}} [\bar{\eta}f'(\bar{\eta}) - f(\bar{\eta})] \tag{3.22}$$

where $\bar{e}(\tau) = e(t)/k$, $\bar{r}_0 = r_0/l^*$, $\bar{\eta} = \bar{y}/C_b \sqrt{\bar{U}/\bar{x}}$, and $C_b = \sqrt{\nu t^*}/l^*$.

According to Equation (3.10), the trajectory of the vortex $\bar{\mathbf{u}}_v$ at the corner is nondimensionalized as,

$$\begin{aligned}
\bar{u}_{vx} &= \bar{x}_v + \bar{e}(\tau)\bar{x}_v + \frac{\bar{y}_v}{2(\bar{x}_v^2 + \bar{y}_v^2)} - \frac{1}{2\bar{y}_v} & \bar{u}_{vy} &= -\bar{y}_v - \bar{e}(\tau)\bar{y}_v + \frac{1}{2\bar{x}_v} - \frac{\bar{x}_v}{2(\bar{x}_v^2 + \bar{y}_v^2)}
\end{aligned} \tag{3.23}$$

According to Equation (3.12), after nondimensionalized, net force $\bar{\mathbf{F}}$ becomes

Potential flow area

$$\begin{aligned}\bar{\mathbf{F}}_{\text{pfa}} &= C_p \left[\frac{\partial \bar{U}}{\partial \tau} + \bar{U} \frac{\partial \bar{U}}{\partial \bar{x}} \right] + C_f C_p |\bar{\mathbf{u}}_r| + (1 - C_p) \mathbf{C}_g \\ \text{where } C_p &= \frac{\rho_f}{\rho_p}, \quad C_f = \frac{18\nu}{kd_p^2}, \quad \mathbf{C}_g = \mathbf{g} \sqrt{\frac{2\pi}{-\Gamma k^3}}\end{aligned}\tag{3.24}$$

Boundary layer area

$$\begin{aligned}\bar{\mathbf{F}}_{\text{bla}} &= C_p \left[\frac{\partial \bar{\mathbf{u}}}{\partial \tau} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} \right] + C_f C_p |\bar{\mathbf{u}}_r| + (1 - C_p) \mathbf{C}_g + \\ &C_p C_{\text{sl}} |\nabla \times \bar{\mathbf{u}}_r|^{-\frac{1}{2}} [\bar{\mathbf{u}}_r \times (\nabla \times \bar{\mathbf{u}})] B + \frac{3}{4} C_p \left[\left(\frac{1}{2} \nabla \times \bar{\mathbf{u}} - \bar{\omega}_d \right) \times \bar{\mathbf{u}}_r \right] + C_{\text{ldw}} \frac{1}{\bar{d}^2} \\ \text{where } C_{\text{sl}} &= \frac{9.66}{\pi d_p} \sqrt{\frac{\nu}{k}}, \quad B = (1 - 0.3314 \bar{\beta}^{1/2}) \exp\left(-\frac{d_p |\nu^* \bar{\mathbf{u}}_r|}{10\nu}\right) + 0.3314 \bar{\beta}^{1/2}, \\ \bar{\beta} &= \frac{d_p}{2l^* |\bar{\mathbf{u}}_r|} |\nabla \times \mathbf{u}|, \quad C_{\text{ldw}} = \frac{3h\nu}{8\pi^2 d_p^2 \rho_p} \frac{t^*}{l^{*3}}\end{aligned}\tag{3.25}$$

A dynamic model for two-phase corner flow has been so far developed theoretically with a chaotic-moving point vortex by the Eulerian-Lagrangian method, in order to trace the responsive performance of the particles, through Equations (3.21) and (3.22) for velocity field of continuous phase, Equation (3.23) for vortex trajectory, and Equations (3.24) and (3.25) for particle movement. The computational flowchart is designed and illustrated in Figure 3.3. The present two-phase model is validated, and the simulation results are discussed in the next section.

Figure 3.3 Computational flowchart

3.3 Validation of two-phase flow model

In order to examine the present two-phase model, a comparison is conducted with the theoretical and experimental works by Julien [170], for the motion of particles within a Rankine point vortex. The main difference between present model and published theoretical work is the modeling method to describe the discrete particles, in which the former uses Lagrangian method to simulate the particle concentration, and the latter Eulerian method.

In the theoretical and experimental works by Julien [170], the motion of dense sediment particles was simulated within a single Rankine point vortex, in which the constant central position and the intensity of the vortex were assumed. The laboratory experiment of a 50 g/L water sediment mixture with fine sediments ($0.0053 < d < 0.0074$ mm) was conducted in water with three liters, where the vortex was induced by a 3" long stirring bar. The fluid velocity was measured at the cross-section surface, and the sediment concentration sampled at several locations in the mixture with 30 mL, with the precision of sediment concentration of 0.1 milligram. For comparison, the present two-phase model is simplified by omitting the effect of the stagnation flow and mirrored vortices for a single Rankine vortex with the stationary center position. The concentration gradient force is added into the right-hand-side of Equation (3.11) due to the higher particle density in published work [170], given by

$$\mathbf{F}_{cg} = -m_p \frac{d}{dt} \left(\frac{D}{C} \nabla C \right) \quad (3.26)$$

where D is the diffusion coefficient, and C the local particle concentration defined as

$$C = \lim_{\Delta r \rightarrow 0} \frac{N(r + \Delta r, t) - N(r, t)}{2\pi r \Delta r l} = \frac{1}{2\pi r l} \frac{\partial N(r, t)}{\partial r} \quad (3.27)$$

where $r = \sqrt{x^2 + y^2}$ represents the distance to vortex center from the particle $\mathbf{P}$, and $N(r, t)$ the number of particles inside the circle with radius r at time t . The model input parameters are the same as those in the theoretical and experimental works by Julien [170], and listed down in Table 3.1.

Table 3.1 Input parameters of the two-phase model for motion of sediment particles in a Rankine point vortex

parameters	symbol	value
radius of vortex core	r_0	0.0096 m
circulation	Γ	$0.041 \text{ m}^2/\text{s}$
ratio of density	C_p	0.366
diameter of particles	d_p	$6.4 \times 10^{-6} \text{ m}$
dynamic viscosity	μ	$1 \times 10^{-3} \text{ Pa} \cdot \text{s}$

The simulations are conducted by programming of MATLAB with time step 0.01s. As illustrated in Figure 3.4, the present two-phase model is examined through the comparison of local particle concentration C in a single Rankine vortex between the presented simulation results and the published theoretical curve and experimental measurement by Julien [170]. The local particle concentration from presented simulation results is evaluated first by a hist bar chart, and then fitted to a curved line, as shown in Figure 3.4. It is found that the simulation results conducted by the presented two-phase model have a great agreement with the previously published theoretical curve represented by the solid line, and the experimental data by scatted points. The difference between the two theoretical results might be due to the statistic method. The hist bar is used to count particle numbers to evaluate average particle concentration in several distant intervals, since particle movements are traced separately by the Lagrangian method. Therefore, the particle concentration in Equation (3.27) is

represented by piecewise line and might not meet high accuracy. However, the tendency of concentration curve is close, and the diffusion force is not required in presented two-phase model. Thereby, it is claimed that the present model can simulate well for two-phase flow with a Rankine vortex involved.

Figure 3.4 Comparison of present theoretical simulation with published theoretical and experimental works [170] for particle distribution in a single Rankine point vortex

3.4 Simulation configuration, results and discussions

By the two-phase model as validated above, the simulations are conducted and then discussed in this section, in order to achieve the optimized energy control strategies for four case studies. The first two imaginary studies investigate the discipline of particle movement without control around a 90-degree corner, detailed by (1) suspending particle dynamics without control in the different initial regions at the corner; (2) suspending particle dynamics without control with the different initial distribution at the corner. The last three relate to practical situation, which are (3) the bioaerosols initially suspending in the air near an

indoor corner; (4) the bioaerosols released from the partial wall and ceiling with a constant rate; (5) the particles, either pollutants or detergents, released within the ventilation outlet with the incoming airflow. The simulation configuration of two-phase corner flow model is introduced in Section 3.4.1, followed by the simulation of particle dynamics with a naturally moving vortex in Section 3.4.2. The simulation results for five case studies are presented from Section 3.4.2 to Section 3.4.6, respectively. The guidelines are finally recommended for the design of control strategies.

3.4.1 **Simulation configuration for case studies**

The simulation configuration is presented in this section. The computational corner zone and configuration of two-phase corner flow model are introduced in Section 3.4.1.1 and Section 3.4.1.2, respectively. The control inputs are designed for the simulation, and several indexes are defined in Section 3.4.1.3 to evaluate the control performance. The optimized energy control strategies are proposed by the orthogonal scheme with two kinds of commonly used control input signals, HSF and PWM, in order to achieve several objectives for different case studies.

3.4.1.1 A computational corner zone for two scenarios

As shown in Figure 3.2 for the computational corner zone, the ongoing air comes from the ventilation outlet located at $(0, l_o)$, lashes towards the x-axis and is approximated by a spin-up model with a central point at (l_o, l_o) . The controllability of the inlet flowrate may be achieved by a flowrate controller to tune the mass flow rate at ventilation outlet or inside ventilation duct. The corner zone is defined as a square with a vertex at the origin $O(0, 0)$ and a length of l_c .

In this work, five case studies are proposed based on the present two-phase corner flow model. The leading two aim to study the discipline of particle movement without control around a 90-degree corner, detailed by (1) suspending particle dynamics initially within different small regions at the corner, as shown in Figure 3.8; (2) suspending particle dynamics initially with different distribution, namely uniform and normal distributions, at the corner, as shown in Figure 3.12. The other three case studies are proposed for the optimization of energy control for practical situations as follows. (1) The particles, such as pollutants, are initially suspended in the air near corner with uniform and normalized distributions. (2) The particles, such as pollutants, are released only from the partial wall and ceiling of the corner with a length of l_m , as shown in Figure 3.2(a), on which enough particle sources are initially distributed uniformly with an interval l_i , and then release particles into the corner zone with a constant frequency λ_p . (3) The particles, either pollutions or detergents, are released from the ventilation outlet located at the position $(0, l_o)$. with an initial concentration, as shown in Figure 3.2(b), and the velocity of releasing particles depends on the airflow velocity at the outlet, determined by the amplitude of the control input. Here, the residual concentration of particles $\bar{C}_{ip}$ is supervised in the corner zone. In general, bioaerosol releasing depends on the biological and environmental characteristics, such as nourishing level, species, temperature, and airflow rate [164, 165]. It is difficult to predict and detect the timing and location of released bioaerosols [164] since the bioaerosol releases in a random manner, but it is relatively easy for the physical aerosols as they are generally measurable. As such, it is unnecessary to control the movement of individual bioaerosols, even if it is

achievable. Therefore, the intensively and continuously releasing aerosol (particle) are simulated, instead of an individual randomly released bioaerosol. As result, the control objective is converted to control of residual concentration for aerosols, instead of control movement of an individual bioaerosol, and the optimized objective is then converted to the optimized residual concentration, instead of the optimized bioaerosol path. For example, once the single bioaerosol is released into the corner zone, it has a larger probability be removed out, if the residual concentration decreases in the intensively released simulation.

3.4.1.2 Configuration of two-phase corner flow model

The configuration of the two-phase corner flow model is tabulated in Table 1. The settings may affect the numerical results from different aspects based on their properties, which may be classified into four categories, namely the particle size, local coefficients, problem-dependent variables, and constants.

Usually the particle size affects the particle movement more or less depending on the friction force $\mathbf{F}_f$, Saffman lift forces $\mathbf{F}_{sl}$, Magnus force $\mathbf{F}_m$, and Van der Waals force $\mathbf{F}_{lvdw}$. The friction force $\mathbf{F}_f = 3\pi d_p \nu \rho_f \mathbf{u}_r$ always minimizes the relative velocity between particle and airflow, in which the amplitude of $\mathbf{F}_f$ significantly influences the particle responding speed if $\mathbf{u}_r \neq \mathbf{0}$ and thus the particle size affect the single-particle trajectory transiently. The particle size also influences the Van der Waals force $\mathbf{F}_{lvdw}$ given in Equation (25), namely the particles adhesion force on the walls. However, the particle size has insignificant influence on the lift force $\mathbf{F}_{sl}$ and Magnus force $\mathbf{F}_m$ due to the low amplitude, as shown in Figure 3.7(a). In the present work, the bioaerosol diameter of 1 μm is

given by the logarithmic average of the various bioaerosol diameter ranging from 0.1 to 10 μm [37]. In addition, the local coefficients, such as the Lifshitz-Van der Waals constant E_L , restitution coefficient e and friction coefficient f , affect the Van der Waals force F_{ldw} and particle collision against walls. However, the present work mainly focuses on control of overall particle concentration inside the corner area with optimized energy consumption. The influence of particle size on the friction force F_f only transiently changes the particle trajectory, such that the trend of overall particle movement remains almost unchanged. Apart from that, the influence of the local coefficients may be ignorable since they are limited within the local boundary layer.

In terms of the problem-dependent parameters, including the circulation Γ , radius of vortex core r_0 , intensity of the original stagnation flow k , and other geometric settings, they are estimated based on a real indoor ventilation situation. Regarding constant input, such as the ratio of density C_p and kinematic viscosity ν , those parameters are given if the water-like bioaerosols are considered within an ideal air.

Table 3.2 Inputs of two-phase corner flow model

Parameter	Symbol	Value
Diameter of particles	d_p	1 μm [37]
Ratio of density	C_p	1.205×10^{-3} [171]
Kinematic viscosity	ν	$1.68 \times 10^{-5} \text{ m}^2/\text{s}$ [171]
Lifshitz-van der Waals constant	E_L	0.6 eV [168]
Restitution coefficient	e	0.7
Friction coefficient	f	0.3 [172]

Circulation	Γ	$-0.789 \text{ m}^2/\text{s}$
Radius of vortex core	r_0	0.05 m
Intensity of the original stagnation flow	k	1 s^{-1}
Length of corner zone	l_c	1 m
Length of moldy area	l_m	0.5 m
Distance between two sources of particle	l_i	0.01 m

3.4.1.3 Control input and evaluation indexes for control performance

As mentioned above, the control strategies are required to be sustainable, repeatable, energy-efficient and easily implementable. The continuously periodic control input is used to optimize the local particle concentration, either bioaerosol or detergent concentration, in which the control activity may remain long-term effective. For example, regarding a randomly released bioaerosol, the optimized control strategy may always remove it out from the corner zone with an optimized probability and energy consumption, because of the repeatable periodic control input, no matter where or when it is released. Two kinds of common control inputs are thus used for simulations to achieve an optimal energy control strategy by the orthogonal scheme, HSF with/without time delay and Pulse Width Modulation PWM with/without time delay, given as

$$\text{HSF} \quad \bar{e}(\tau) = \begin{cases} \bar{e}_m, & \tau \geq \delta \\ 0, & \tau < \delta \end{cases} \quad (3.28)$$

$$\text{PWM} \quad \bar{e}(\tau) = \begin{cases} \bar{e}_m, & \delta + nT_s \leq \tau \leq \delta + nT_s + T_{\text{on}}, n = 0, 1, 2, 3 \dots \\ 0, & \text{else} \end{cases} \quad (3.29)$$

where $\bar{e}_m$, δ and T_s represent the amplitude, time delay and period respectively.

$T_{on} = \eta T_s$ is the working duration of the control input, where η is duty factor.

Table 3.3 Levels of control input parameters

Input parameters	Level 1	Level 2	Level 3	Level 4	Level 5
T_s	0.5	1	1.5	2	2.5
$\bar{e}_m$	0.05	0.1	0.15	0.2	0.25
η	0.15	0.3	0.45	0.6	0.75
δ	0	5	-	-	-

The amplitude of the control input $\bar{e}_m$ is given maximumly by 25% since it indicates the airflow rate at ventilation outlet, which significantly affects energy consumption and comfort level to the residents, especially in an air-conditioned room. Therefore, according to the orthogonal scheme, five levels for each input parameter are proposed to achieve an optimal energy strategy, as detailed in Table 3.3. However, the time delays δ of 0 and 5 are given in each function, rather than a variable, since the time delay doesn't make a significant impact on a continuous process. $\delta = 0$ means that control input starts working as soon as particles are released (no time delay in the control input), while $\delta = 5$ is chosen to form an initial accumulation for the particles released in the corner zone. Therefore, ten sets of trials for HSF and 50 sets of trials for PWM are proposed as the control inputs via the orthogonal scheme, detailed in Table 3.4 and Table 3.5 in supporting information.

According to Equation (3.22), different control inputs result in different trajectories of the vortex center. Two representative control inputs, HSF with ($\bar{e}_m = 0.25$ and $\delta = 5$), PWM with ($\bar{e}_m = 0.1$, $T_s = 2.5$, $\eta = 0.6$ and $\delta = 0$), are

illustrated their influences on the trajectories of vortex center, as shown in Figure 3.5, in which the given control inputs make changes on both period and amplitude of vortex movement.

Table 3.4 Design of control input HSF by orthogonal scheme

Simulation No.	HSF		Simulation No.	HSF	
	e_m	δ		e_m	δ
1	0.05	0	31	0.05	5
2	0.10	0	32	0.10	5
3	0.15	0	33	0.15	5
4	0.20	0	34	0.20	5
5	0.25	0	35	0.25	5

Table 3.5 Design of control input PWM by orthogonal scheme

Simulation No.	PWM				Simulation No.	PWM			
	T_s	e_m	η	δ		T_s	e_m	η	δ
6	2.00	0.25	0.15	0	36	2.00	0.25	0.15	5
7	0.50	0.10	0.30	0	37	0.50	0.10	0.30	5
8	2.50	0.15	0.15	0	38	2.50	0.15	0.15	5
9	0.50	0.15	0.45	0	39	0.50	0.15	0.45	5
10	2.00	0.15	0.60	0	40	2.00	0.15	0.60	5
11	1.00	0.10	0.60	0	41	1.00	0.10	0.60	5
12	1.00	0.15	0.75	0	42	1.00	0.15	0.75	5
13	2.00	0.05	0.30	0	43	2.00	0.05	0.30	5
14	1.50	0.15	0.30	0	44	1.50	0.15	0.30	5
15	1.00	0.20	0.15	0	45	1.00	0.20	0.15	5
16	1.00	0.25	0.30	0	46	1.00	0.25	0.30	5
17	1.00	0.05	0.45	0	47	1.00	0.05	0.45	5
18	2.50	0.10	0.75	0	48	2.50	0.10	0.75	5
19	0.50	0.05	0.15	0	49	0.50	0.05	0.15	5
20	2.00	0.10	0.45	0	50	2.00	0.10	0.45	5
21	1.50	0.05	0.75	0	51	1.50	0.05	0.75	5
22	2.50	0.20	0.30	0	52	2.50	0.20	0.30	5
23	1.50	0.10	0.15	0	53	1.50	0.10	0.15	5
24	2.50	0.05	0.60	0	54	2.50	0.05	0.60	5
25	0.50	0.25	0.75	0	55	0.50	0.25	0.75	5
26	1.50	0.25	0.60	0	56	1.50	0.25	0.60	5
27	2.50	0.25	0.45	0	57	2.50	0.25	0.45	5
28	1.50	0.20	0.45	0	58	1.50	0.20	0.45	5
29	2.00	0.20	0.75	0	59	2.00	0.20	0.75	5
30	0.50	0.20	0.60	0	60	0.50	0.20	0.60	5

Figure 3.5 Comparison of trajectory of vortex centres subject to zero control input and two representative control inputs

Definition of evaluation indexes

The energy efficiency γ_e is assessed by the ratio of the relative difference in residual particle concentration and energy consumption E , which indicates the capacity to influence residual particle concentration from unit energy consumed, as defined by

$$\gamma_e = \frac{\gamma_c}{E} = \frac{1}{E} \frac{\bar{C}_{ipc} - \bar{C}_{ipn}}{\bar{C}_{ipn}} \quad (3.30)$$

where γ_c is the control efficiency, $\bar{C}_{ipc}$ and $\bar{C}_{ipn}$ are the residual particle concentration with a forced moving vortex namely $\bar{e}(\tau) \neq 0$, and a natural one namely $\bar{e}(\tau) = 0$.

It is noted that energy efficiency γ_e depends on the interested time due to fluctuation. The average γ_e is thus used to evaluate the energy efficiency upon a given duration, by $\xi_{ee} = \int \gamma_e d\tau / t_s$, where t_s indicates the terminal time. The

negative value of ξ_{ee} indicates the positive effort by consumed energy on the reduction of the residual particle concentration until the given time.

Based on the above definitions, the control performance is evaluated by the loss function, as formulated below,

$$\Phi = \max \text{ or } \min \{ \lambda \bar{\xi}_{ee} + \bar{\xi}_{C_\tau} \} \quad s.t. \quad 0 \leq \bar{\xi}_{ee} \leq 1, \quad 0 \leq \bar{\xi}_{C_\tau} \leq 1 \quad (3.31)$$

where $\bar{\xi}_{ee} = \xi_{ee} / \max\{|\xi_{ee}|\}$ is the normalized average of the energy efficiencies γ_e in a certain duration, $\bar{\xi}_{C_\tau}$ the normalized duration when the particle concentration is larger than a value C_τ specified by environmental requirement. λ is the weight factor to balance the significance between $\bar{\xi}_{ee}$ and $\bar{\xi}_{C_\tau}$. The first part $\bar{\xi}_{ee}$ in the loss function, aims to evaluate the global energy efficiency γ_e , and the second part $\bar{\xi}_{C_\tau}$ to evaluate the duration when the environmental state is at a high level of particle concentration. Here, the maximum or minimum of the loss function selected depends on the control objectives. If less residual particle concentration is expected in the corner zone, such as removal of pollutants, the minimum is imposed on the loss function Φ . Otherwise, the maximum of the loss function Φ is considered, such as reserve of detergents.

The flow chart of the control design via orthogonal methods is schematically shown in Figure 3.6.

Figure 3.6 Schematic flow chart of controller design to optimize residual particle concentration in a gas-particle corner flow via orthogonal design

3.4.2 Case study I: Suspending particle dynamics without control initially in different regions at corner

An imaginarily suspending particle dynamics with a natural moving vortex, namely $\bar{e}(t) = 0$, is simulated to study the particle movements by the influence of the corner flow in the corner zone based on the proposed two-phase model. A single particle dynamic initially released in the boundary layer is simulated first, in order to study the influence of each force in Equations (3.24) and (3.25). After that, the dynamics of a cluster of particles is investigated by particles initially suspended in different zones of the moldy area.

A single particle is initially released at $(0.5l_m, 5d_p)$ freely, where is inside the boundary layer area. Figure 3.7(a) shows the variation of amplitudes of different forces with non-dimensional time that a particle is conducted in the boundary layer, and Figure 3.7(b) shows the particle trajectory. As illustrated in these pictures, if the particle reaches close to the wall surface, the Van der Waals

force increases sharply and dominates the particle movement. The particle experiences several bounces due to collision to the wall with a gradually decreased intensity. After that, it starts to slide on the wall surface under the influence of Van der Waals force.

Figure 3.7 Evolution of (a) different forces imposed on a single particle, and (b) particle trajectory in boundary layer

In order to study dynamics of a cluster of imaginarily suspending particles, the corner area is divided into nine uniform partitions, numbered as Zone 1 to 9 as shown in Figure 3.8. The particles are initially distributed in each zone with a uniform interval as $l'_i = 5 \times 10^{-3}$ m. Two representative evolutions of particle movement in Zones 5 and 7 are illustrated at several dimensionless time τ respectively in Figure 3.9 and Figure 3.10.

The stagnation flow dominates the motion of the particles initially located in Zones 1, 2 and 3, and drives the particles out of the corner zone quickly, since they are relatively far away from the center. However, the particles initially located in the other zones are more influenced by the vortex. For example, it is shown in Figure 3.9 that, when the vortex moves towards the anti-y-axis

direction, the particles initially located in Zone 5 tend to approach to the x -axis. However, as the vortex moves towards the anti- x -axis direction, the partial particles are conveyed towards the corner, as shown in Figure 3.9 (b). This phenomenon makes some particles left at the corner.

Figure 3.8 Division of the particle suspending area

Figure 3.9 Evolution of particle movement in Zone 5 at (a) $\tau = 0.5$, (b) $\tau = 2.3$, (c) $\tau = 5$.

Figure 3.10 Evolution of particle movement in Zone 7 at (a) $\tau = 0.5$, (b) $\tau = 2.3$, (c) $\tau = 5$

Figure 3.11 Variation of residual particle concentration with dimensionless time τ

As shown in Figure 3.9 and 3.10, it is observed that the particles are removed much more difficultly out from the corner in the zero-control condition, if the particles are initially placed closer to the vertex of the corner. The similar experimental phenomenon reveals that usually the indoor particle concentration at the corner is higher than that in the other area, and it is influenced significantly by the airflow disturbance [135, 159]. Moreover, the similar phenomenon is found in the open literature [135], in which the indoor particles were monitored experimentally in a naturally ventilated meeting room, and the indoor particle

concentration peaked at the corner due to vertexes capturing the particles, generated by local airflow disturbance. Hence, a desired residual particle concentration may be achieved by control of the vortex trajectory with a properly designed control input.

In addition, the variation of residual particle concentrations in all the 9 zones is plotted in Figure 3.11. Particles originally located in Zones 1, 4, 5, 8 and 9 have a much higher residual concentration than the others. On the contrary, the particles initially located in Zones 3, 6, and 9 are removed easily from the corner, since they are distributed in the downwind location and far away from the corner.

3.4.3 Case study II: Suspending particle dynamics without control by different initial distributions at corner

Two kinds of different particle initial distribution, uniform and normal distributions, are considered for discussing the influence of the initial particle concentration in this subsection.

As depicted in Figure 3.12 (a) and (b), the particles are initially generated all over the moldy area uniformly in the first picture and normally in the second one, which the total number of the initial particles is the same. The normalized initial particle locations are generated by a stand normal function with zero average distance towards the original point and 1 standard deviation.

The comparison of the residual particle percentage between the two different initial distribution is shown in Figure 3.12, in which the particles with a normalized one are to be removed more difficult from the corner due to higher particle concentration near the original point. In other words, if the particles are

more located close to the corner point, it is more difficult to remove them outwards the corner area, only relying on a constant inlet airflow rate, namely nature ventilation. The conclusion is exactly the same as what is drawn in Case Study I as discussed above.

Figure 3.12 Initial distribution of particles in moldy area

Figure 3.13 Variation of residual particle percentage with different initial distributions

3.4.4 Case study III: Optimized energy control for bioaerosols initially suspended at indoor corner with different distributions

This case study refers to the corner zone polluted by the bioaerosols with either uniform or normal distributions. In other words, it is assumed theoretically that the particles suspend initially in the entire mold area, either as a fixed space interval at $l_i = 0.01$ m each other or as a normal distribution with the mean at $x = 0$ and $y = 0$. The particle concentration is then controlled for the objective of an acceptable residual particle concentration with an optimized energy consumption, computed by Equation (3.19). For achieving this control objective, the control inputs for trial-and-error simulations are discussed in Section 3.4.1, and further detailed in Table 3.4 and Table 3.5.

Based on the different requirements of the bioaerosol concentration for the various rooms, three indexes are selected, namely the 30%, 10% and 5% of the residual particle concentration over the initial concentration, respectively, in order to evaluate the effect of the influence between the airflow and the particle movement.

Uniform distribution

Figure 3.14 Energy consumption when the residual particle concentration is reduced to (a) 30%, (b)10%, and (c) 5% with HSF control inputs

The simulation data with a HSF input is plotted in Figure 3.14, in which the circle spots represent the different simulations with various control inputs and the square one represents the simulation without control.

Each point in Figure 3.14 represents one simulation result with the control inputs listed in Tables 3.3 to 3.5. The multiple energy consumptions at the same time are calculated based on different control inputs. It is indicated that the control inputs in these simulations can reduce the residual particle concentration to a given percentage, but consume different energy due to different parameters in each control input. The x axis in each figure indicates the time instant if the residual particle concentration reduces to certain levels, e.g. 30%, 10% or 5% of the initial concentration. A lower x value in those figures gives a stronger particle removal ability. In general, the simulation with a higher energy consumption, namely y value in Figure 3.14, meets the requirement of residual concentration more quickly. As shown in Figure 3.14, the energy consumption becomes a trade-off with the speed to reduce the residual particle concentration to a certain level under the most circumstances. In other words, the particles tend to be removed faster with increase of the amplitude of control input. The loss function defined in Equation (3.31) is a criterion to evaluate the energy consumption and the speed of particles removal from the corner, in which Φ is minimized as lower residual particle concentration is desired for this scenario. In addition, λ is the weight factor that is determined by the real requirement, such as the required bioaerosol concentration and the cost of the energy consumption. For example, $\lambda = 1$ means

that the efficiency of particle remove and the cost of the energy consumption are equally important, while, $\lambda < 1$ means that the efficiency of particle removal values more than the cost of the energy consumption. In the following, λ is assigned as $0.8 \leq \lambda \leq 1.2$.

Figure 3.15 Selection of optimized HSF control input when residual particle concentration is reduced to 30%.

As illustrated in Figure 3.15, only the 15th and 25th simulations meet the requirements of the minimized weight function as $0.8 \leq \lambda \leq 1.2$, where the corresponding control inputs are $\delta = 0$, $e_m = 0.15$ and $\delta = 0$, $e_m = 1$, as listed in Table 3.4. Other spots are not located in the feasible region, indicating that no more optimal solutions are found under such circumstance. The similar results are obtained when the objective residual particle concentrations reach 10% and 5%, as shown in Figure 3.16.

(a)

(b)

Figure 3.16 Selection of optimized HSF control input when residual particle concentration is reduced to (a) 10% and (b) 5%.

(a)

Figure 3.17 Selection of optimized PWM control input with initially uniform distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.

In terms of the PWM control input, the same pictures are drawn for obtaining optimal residual particle concentration with considering the energy consumption. All the evaluate parameters, such as λ and controlled residual particle levels, are the same as the ones mentioned above. The results are shown in Figure 3.17, in which the 23rd simulation is the unique optimal solution that meets the requirements, as $T_s = 2.5$, $e_m = 0.1$, $\eta = 0.75$ and no delay.

Normal distribution

Similar simulations are completed as the particles are normally distributed initially in the corner zone. The results are plotted in Figure 3.18, in which the optimal residual particle concentration is obtained by the HSF control input with the same parameters as the initially uniform distribution, namely $\delta = 0$, $e_m = 0.15$ and $\delta = 0$, $e_m = 0.1$.

When it comes to the PWM control input, the simulation results are shown in Figure 3.19, in which the 23rd simulation is also the unique optimal solution that meets the requirements, as $T_s = 2.5$, $e_m = 0.1$, $\eta = 0.75$ and no delay.

(c)

Figure 3.18 Selection of optimized PWM control input with initially normal distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.

(a)

(b)

(c)

Figure 3.19 Selection of optimized PWM control input with initially normal distribution when residual particle concentration is reduced to (a) 30%, (b) 10%, and (c) 5%.

3.4.5 Case study IV: Optimized energy control for bioaerosols released from the partial ceiling and wall

This case study refers to the walls at the indoor corner polluted by the microorganism that continuously aerosolizes or releases bioaerosols into the corner zone, as shown in Figure 3.2(a). Here, the continually released bioaerosols simulate the saturated releasing and their residual concentration indicates the probability of bioaerosols remaining inside the corner zone. The control activities work for the system to get a least residual particle concentration with optimized energy consumption, which is expressed as the minimum of the loss function in Equation (3.31). The evolution of particle movement with zero control input is plotted in Figure 3.20 at specified time. As shown in the figure, the particles tend to move with the vortex and form a moving circle around the vortex center. The stirring effect of the vortex conveys the particles away from the axes, and the particles are then transported out of the corner area by the airflow.

Figure 3.20 Evolution of movement for particle released from partial wall and ceiling with $\bar{e}_m = 0$ at (a) $\tau = 0$, (b) $\tau = 2$, (c) $\tau = 5$, (d) $\tau = 10$, (e) $\tau = 15$, (f) $\tau = 20$

As demonstrated in Figure 3.21(a), the residual particle concentration C_{ip} goes through a fluctuation state with the nondimensional time τ . Figure 3.21(b) is plotted for comparison of energy efficiency γ_e to residual particle concentrations subject to different HSF inputs with $\delta = 0$, in which the larger fluctuation is conducted by the higher amplitude of HSF. However, as shown in

this figure, control performance is not always improved by the control activities since control efficiency γ_c sometimes turns positive.

(a) Residual concentration C_{ip}

(b) Control efficiencies γ_c

Figure 3.21 Comparison of (a) residual concentration C_{ip} and (b) control efficiency γ_c subject to different HSFs with $\delta = 0$

It is obvious that the simulations with PWM inputs cannot cover all the combinations of the three parameters, T_s , $\bar{e}_m$ and η . Therefore, it is necessary to study the influence of each input parameter on the loss function Φ , for confirmation of the optimized control via the analysis of the orthogonal design scheme.

(a) $\lambda_2 = 0.8$ and $C_\tau = 30$

(b) $\lambda_2 = 0.8$ and $C_\tau = 30$

(c) $\lambda_2 = 1.2$ and $C_\tau = 30$

Figure 3.22 Variation of loss function Φ with different control inputs at different weight factors (a) $\lambda_2 = 0.8$, (b) $\lambda_2 = 1$, and (c) $\lambda_2 = 1.2$

The optimized control input is determined by the comparison of loss function ϕ in Equation (3.31) subject to different weight factors via the analysis of the orthogonal design scheme. As shown in Figure 3.22, the 19th simulation with

($\bar{e}_m = 0.05$, $T_s = 0.5$, $\eta = 0.15$ and $\delta = 5$) is the optimized control input that minimizes the loss functions ϕ if $\lambda_1 = 0.8$, 1 and 1.2. The 26th simulation with ($\bar{e}_m = 0.25$, $T_s = 1.5$, $\eta = 0.6$ and $\delta = 0$) maximizes the loss function Φ , leading to the worst control performance.

Table 3.6 Average of loss function $\Phi_{n,avg}$ at each parameter level when $C_\tau = 30$ for Case Study IV

Input parameters	λ_1	$\Phi_{1,avg}$	$\Phi_{2,avg}$	$\Phi_{3,avg}$	$\Phi_{4,avg}$	$\Phi_{5,avg}$
T_s	0.8	0.1893	0.1259	0.2946	0.0904	0.2284
$\bar{e}_m$	0.8	-0.2259	0.0754	0.2700	0.3909	0.4182
η	0.8	-0.0509	-0.0173	0.2298	0.3212	0.4457
δ	0.8	0.2219	0.1495	-	-	-
T_s	1.0	0.1321	0.0824	0.2548	0.0393	0.1885
$\bar{e}_m$	1.0	-0.3449	0.0263	0.2423	0.3700	0.4034
η	1.0	-0.1179	-0.0702	0.1876	0.2840	0.4136
δ	1.0	0.1789	0.0999	-	-	-
T_s	1.2	0.0749	0.0388	0.2151	-0.0119	0.1485
$\bar{e}_m$	1.2	-0.4639	-0.0228	0.2146	0.3492	0.3885
η	1.2	-0.1848	-0.1232	0.1454	0.2467	0.3814
δ	1.2	0.1359	0.0503	-	-	-

The average values of the loss functions $\Phi_{n,avg}$ at the parameter level n are listed in Table 3.6 for the four control inputs, namely the period T_s , amplitude $\bar{e}_m$, duty factor η and time delay δ , in which $\Phi_{n,avg}$ represents the average of the loss function Φ at the various possible combinations of the other three parameters if one of the four parameters is given at the level n . For example, $\Phi_{3,avg} = 0.0263$ at the row 6 and the column 5 is given by the average of Φ at all the possible combinations of other three variables T_s , η and δ according to

Table 3.5, such as Simulations 8, 9, 10, 12, 14, 38, 39, 40, 42 and 44, when $\bar{e}_m = 0.15$ is fixed at the level 3 in Table 3.4, where $\lambda_1 = 1.0$.

As shown in Table 3.3, the potential combination of control inputs to minimize loss function Φ is T_s at Level 4, $\bar{e}_m$ at Level 1, η at Level 1 and δ at Level 2, namely $(T_s = 2, \bar{e}_m = 0.05, \eta = 0.15, \delta = 5)$ for $\lambda_1 = 0.8, 1$ and 1.2 . By additional simulation with this control input, the loss functions ϕ produce the values of -0.2385, -0.3884 and -0.5383 for $\lambda_1 = 0.8, 1$ and 1.2 respectively, which are larger than those in 19th Simulation. Therefore, the set of control input, $(T_s = 0.5, \bar{e}_m = 0.05, \eta = 0.15$ and $\delta = 5)$, is the optimized energy control strategy Case Study IV, namely the bioaerosols released from the partial ceiling and wall with a constant rate.

As a result, the set of control input, $(T_s = 0.5, \bar{e}_m = 0.05, \eta = 0.15$ and $\delta = 5)$, is the optimized energy control strategy for the first scenario. The control decreases the residual bioaerosol concentration by 1.31%, compared with natural ventilation. It is noteworthy that the selected control input may not pursue an extreme reduction in residual bioaerosol concentration. However, it is the optimal combination to balance energy consumption and concentration reduction, which is very significant to a long-term continuous process in real applications.

3.4.6 Case study V: Optimized energy control for bioaerosols/detergents released from ventilation outlet

Here, the particles, representing either pollutions or detergents, are released from the ventilation outlet located at the position $(0, l_o)$ with an initial concentration

of about $6000 / \text{m}^3$, as shown in Figure 3.2(b). This scenario simulates the situation of polluted inlet air discharged into the indoor environment due to the microorganism growing inside the ventilation ducts, or a sprayer installed around the ventilation outlet generating the detergent particles to restrain the growth of the microorganism on the indoor corner. The velocity of releasing particles depends on the airflow velocity at the outlet, determined by the amplitude of the control input.

The evolution of the particle movement is illustrated in Figure 3.23 at non-dimensional time $\tau = 0.5, 2, 5, 10, 15$, and 20 , with the naturally moving vortex, namely, $\bar{e}_m = 0$. As shown in Figure 3.23, the particles tend to move with the vortex after flowing into the corner zone and form a moving circle around the vortex center. The stirring effect of vortex attracts the particles moving around it. However, once the particles move far away from the vortex center, they will be transported away from the corner zone via the streamline near the x -axis direction. The desired control objectives are to minimize the residual particle concentration such as pollutants, or maximize the residual particle concentration such as detergent, with optimized energy consumption. Here, loss function Φ in Equation (3.31) is specified as $\Phi_p = \min\{\lambda \bar{\xi}_{ee} + \bar{\xi}_{C\tau}\}$ with weight factor λ_2 for pollutants, and $\Phi_d = \max\{\lambda \bar{\xi}_{ee} + \bar{\xi}_{C\tau}\}$ with λ_3 for detergent respectively. It is well known that the higher amplitude of control input accelerates the particle removal inside the corner zone, while it increases the energy consumption and the number of released particles.

Figure 3.23 Evolution of movement for particles released within ventilation

outlet with $\bar{e}_m = 0$ at (a) $\tau = 0.5$, (b) $\tau = 2$, (c) $\tau = 5$, (d) $\tau = 10$,

(e) $\tau = 15$, and (f) $\tau = 20$

(a) Residual concentration C_{ip}

(b) Control efficiency γ_c

Figure 3.24 Comparison of (a) residual concentration C_{ip} and (b) control efficiency γ_c subject to different HSFs with $\delta = 0$

As depicted in Figure 3.24(a), the comparison of residual concentration C_{ip} subject to different HSF inputs with $\delta = 0$. As shown in this figure, the residual concentration C_{ip} behaves as a fluctuation with the nondimensional time τ , in which the amplitude of the fluctuation remains almost stable.

(a) $\lambda_2 = \lambda_3 = 0.8$, $C_\tau = 48$

(b) $\lambda_2 = \lambda_3 = 1$, $C_\tau = 48$

(c) $\lambda_2 = \lambda_3 = 1.2$, $C_\tau = 48$

Figure 3.25 Variation of loss function Φ with different control inputs at

different weight factors (a) $\lambda_2 = \lambda_3 = 0.8$, $C_\tau = 48$, (b)

$\lambda_2 = \lambda_3 = 1$, $C_\tau = 48$ and, (c) $\lambda_2 = \lambda_3 = 1.2$, $C_\tau = 48$.

The optimized control input is determined by the comparison of loss function Φ in Equation (3.31), taking minimum for pollutants and maximum for detergents, subject to different weight factor $\lambda_2 = \lambda_3 = 0.8$ and the desired

residual particle concentration $C_\tau = 48$ via the analysis of the orthogonal design scheme. As plotted in Figure 3.25, the 48th simulation with a PWM input as ($\bar{e}_m = 0.1$, $T_s = 2.5$, $\eta = 0.75$ and $\delta = 5$) is the optimal control input that minimizes the loss functions ϕ as $\lambda_2 = \lambda_3 = 0.8$, 1 and 1.2, and $C_\tau = 48$. However, the 25th simulation with a PWM input as ($\bar{e}_m = 0.25$, $T_s = 0.5$, $\eta = 0.75$ and $\delta = 0$) reaches maximum for $\lambda_2 = \lambda_3 = 0.8$ and 1, and $C_\tau = 48$. The 19th simulation with a PWM input as ($\bar{e}_m = 0.05$, $T_s = 0.5$, $\eta = 0.15$ and $\delta = 0$) reaches maximum for $\lambda_2 = \lambda_3 = 1.2$, and $C_\tau = 48$.

Table 3.7 Average of loss function $\Phi_{n,avg}$ at each parameter level when $C_\tau = 48$

Input parameters	λ_2	λ_3	$\Phi_{1,avg}$	$\Phi_{2,avg}$	$\Phi_{3,avg}$	$\Phi_{4,avg}$	$\Phi_{5,avg}$
T_s	0.8	0.8	0.5520	0.4508	0.4539	0.4885	0.3729
$\bar{e}_m$	0.8	0.8	0.4525	0.3504	0.3891	0.5062	0.6200
η	0.8	0.8	0.3399	0.4029	0.4656	0.5315	0.5783
δ	0.8	0.8	0.6872	0.2400	-	-	-
T_s	1.0	1.0	0.6028	0.4969	0.5012	0.5361	0.4157
$\bar{e}_m$	1.0	1.0	0.5474	0.4002	0.4240	0.5352	0.6459
η	1.0	1.0	0.3938	0.4517	0.5125	0.5741	0.6207
δ	1.0	1.0	0.7700	0.2511	-	-	-
T_s	1.2	1.2	0.6536	0.5429	0.5485	0.5838	0.4584
$\bar{e}_m$	1.2	1.2	0.6422	0.4500	0.4589	0.5642	0.6718
η	1.2	1.2	0.4476	0.5005	0.5594	0.6167	0.6630
δ	1.2	1.2	0.8527	0.2622	-	-	-

The similar process is necessary to study the influence of each parameter on Φ_p and Φ_d , for the confirmation of the above optimized control via the analysis of the orthogonal design scheme, as explained in the first scenario. The progress

is conducted by Table 3.7, where $\Phi_{n,avg}$ are the average values of the loss functions at the n th parameter level.

As shown in Table 3.7, the potential combinations of control inputs to maximize or minimize the loss function Φ_{pp} are listed below.

- (a) The loss function Φ_{pp} may be minimized if $T_s = 2.5$ at Level 5, $\bar{e}_m = 0.1$ at Level 2 and $\eta = 0.15$ at Level 1 and $\delta = 5$ for $\lambda_2 = \lambda_3 = 0.8, 1$ and 1.2 , and $C_\tau = 48$;
- (b) The loss function Φ_{pp} may be maximized if $T_s = 0.5$ at Level 1, $\bar{e}_m = 0.25$ at Level 5, $\eta = 0.75$ at Level 5, and $\delta = 0$ for $\lambda_2 = \lambda_3 = 0.8, 1$ and 1.2 , and $C_\tau = 48$.

The loss functions Φ_{pp} reach 1.8418, 2.2977, 2.7536 at condition (a) for $\lambda_2 = \lambda_3 = 0.8, 1$ and 1.2 , and $C_\tau = 48$ respectively, which are larger than those in the 48th simulation. It is also found that $\bar{\xi}_{ee}$ in Φ_{pp} remain positive and are larger than those in the 48th simulation, but $\bar{\xi}_{C_\tau}$ are smaller, meaning that the imposed control activities are not able to reduce the residual pollutant concentration if they are released from the ventilation outlet. Therefore, for this case, the optimal choice is natural ventilation, namely $\bar{e}_m = 0$. In terms of the above condition (b), Φ_{pp} are exactly the same as the 25th simulation. It is thus concluded that for the case of reservation detergent in the corner zone, the optimized control inputs are PWM with ($\bar{e}_m = 0.25, T_s = 0.5, \eta = 0.75$ and $\delta = 0$) for $\lambda_2 = \lambda_3 = 0.8$ and 1 ,

and $C_\tau = 48$, and $(\bar{e}_m = 0.05, T_s = 0.5, \eta = 0.15 \text{ and } \delta = 0)$ $\lambda_2 = \lambda_3 = 1.2$, and $C_\tau = 48$.

It is thus concluded that for the case of reservation detergent in the corner zone, the optimized control inputs are PWM with $(\bar{e}_m = 0.25, T_s = 0.5, \eta = 0.75 \text{ and } \delta = 0)$ for $\lambda_2 = \lambda_3 = 0.8$ and 1, and $C_\tau = 48$, and $(\bar{e}_m = 0.05, T_s = 0.5, \eta = 0.15 \text{ and } \delta = 0)$ for $\lambda_2 = \lambda_3 = 1.2$ and $C_\tau = 48$. The former input increases the average detergent concentration by 9.37%, and the later one by 0.46% but it consumes much less energy. It is noted that the optimized control inputs don't pursue an extreme improvement in residual particle concentration. However, they are the optimal choices to balance the energy consumption and concentration increase.

3.4.7 **Recommended guidelines for optimal operation conditions**

Recommended guidelines for optimal operation conditions

Based on the simulation results, a small variation of the airflow rate from the ventilation outlet contributes to reducing the residual concentration of bioaerosols that are originally released from the corner, or to increasing the residual concentration of detergents that are released from the ventilation outlet. The optimal operating conditions are summarized in Table 3.8 for the present scenarios, and they depend on different requirements of environmental conditions and energy consumptions. Usually the larger amplitude of control input results in a higher control efficiency of the bioaerosol removal and detergent reservation in the corner zone. However, larger amplitude also leads to more energy consumption. If the strict requirement of air quality is pursued at the

indoor corner, a control input with a large amplitude is imposed on the airflow rate from the ventilation outlet. Moreover, the weight factor λ and required pollution/detergent concentration C_r are adjustable in the loss function Φ for design of optimal control strategies to meet different requirements.

Table 3.8 Summary of optimal operating conditions for Cases IV and V

λ		Optimal operating conditions
Case IV	Pollutant $\lambda_1 = 0.8, 1, \text{ and } 1.2$	$T_s = 0.5$, $\bar{e}_m = 0.05$, $\eta = 0.15$ and $\delta = 5$
Case V	Detergent $\lambda_2 = \lambda_3 = 0.8, 1$	$\bar{e}_m = 0.25$, $T_s = 0.5$, $\eta = 0.75$ and $\delta = 0$
	Detergent $\lambda_2 = \lambda_3 = 1.2$	$\bar{e}_m = 0.05$, $T_s = 0.5$, $\eta = 0.15$ and $\delta = 0$
	Pollutant $\lambda_2 = \lambda_3 = 0.8, 1, 1.2$	$\bar{e}_m = 0$

The continuity and time delay of the control input depends on different control objectives, either the decrease of pollutant concentration or the increase of detergent concentration. In the scenario one, the preferred PWM control has a period close to the half that of the point vortex movement, and a relatively small duty factor to reduce the energy consumption. A time delay is preferred to make an initially accumulation of pollutant for a high energy efficiency. In the scenario two however, the optimized control input tends to have a shorter period, higher duty factor, and zero-time-delay to release more detergent into the corner zone.

Apart from that, it is also observed that cleanliness of the ventilation is essential to get rid of bioaerosol pollution at an indoor corner. As shown in Figure 14, any control input of the airflow rate of the ventilation always fails to reduce the pollutant concentration at corner, if the pollutant source is seeded inside the ventilation outlet.

3.5 Remarks

A two-phase corner flow model including a trajectory controllable moving vortex has been developed for analysis of the particle dynamics at the indoor corner. Based on the present model, a control strategy is developed to reduce the bioaerosol concentration at the indoor corner with optimized energy consumption. The two-phase flow model is validated by comparison of similar multi-phase model and experiments with a stationary vortex, in which good agreements are achieved. Moreover, the present working platform, consisting of the two-phase model with moving vortex and control strategy, provides a novel energy-efficient way to improve the indoor air quality, by taking advantage of the controllable airflow pattern from ventilation, instead of using extra air cleaning machines or human force. Base on the simulation results, particles close to the corner vertex are more challenging to be removed out of a corner area. In addition, the incoming airflow from ventilation outlet with a Pulse Width Modulation controller is feasible to improve the local indoor air quality without human operation and the controller is more energy efficient if the control parameters are well designed, such as low amplitude, proper duty factor, period and time delay, is more. Furthermore, the proposed platform will broaden the techniques for addressing the bioaerosol polluting problem, since it may either remove the

dispersed pollutants at the indoor corner, or spray the detergent to restrain the bioaerosol growth with optimized energy efficiency.

Chapter 4 Development of Neural Network Model Predictive Control (NN-MPC) controller of particle concentration for two-phase laminar corner flow with optimized energy consumption

In this chapter, a novel NN-based control method is proposed to optimize the bioaerosol concentration at an indoor corner via a gas-particle laminar corner flow with energy efficiency. The two-phase corner flow area is divided into three zones, recirculation, paralleled flow and ambient flow zones, among which the recirculation zone dominates the local particle concentration at the corner since particles in this zone are trapped within it. The profile and the flow center of the recirculation zone are determined mathematically by the minimum max flux principle of the fluid and grid search method. After that, the characteristics of the transient profile of the recirculation zone with laminar flow assumption are then studied by a NN model after wavelet transform, in which the dataset is collected from the simulation by the Eulerian-Lagrangian scheme. Moreover, a model predictive controller (MPC) is designed to achieve an optimal profile of recirculation zone with minimum energy required on the effort on controlling the airflow rate from the ventilation outlet based on the proposed linearized NN model. Finally, the method is employed to the improvement of the local bioaerosol concentration at indoor corner through a flow-rate-controllable air inlet located at ceiling with optimal energy consumption. The statement of the problem is given first in Section 4.1, followed by the formulation of two-phase flow at the corner area in Section 4.2. The formulation of the recirculation zone at the corner is presented in the subsequent section. The simulation configuration,

results and discussion are elaborated in Section 4.4, following by remarks in Section 4.5.

4.1 Problem statement

Figure 4.1 Schematics of (a) the indoor corner with bioaerosol pollution, and (b) computation domain of the two-phase corner flow model

The present indoor corner flow is illustrated schematically in Figure 4.1(a), specified for the area around the edges of the ceiling. It may be simplified as a 2D right angle due to the infinite length in the horizontal direction, namely along the z -axis. As shown in Figure 4.1(b), the computational domain for corner flow is defined by a right angle with two semi-infinite sides, and the fresh air is exhausted into the corner area from the ventilation outlet located at the top border of the domain. Apart from that, the bioaerosols/detergents are freely released around the corner, and then driven by the airflow. Theoretically, several assumptions are made as follows: (1) incompressible laminar airflow considered; (2) no collision among particles due to the low density; and (3) no influence of particle movement on airflow due to the small particle size.

4.2 Modeling of gas-particle laminar corner flow

In this section, the modelling of gas-particle laminar corner flow dynamics is introduced in Section 4.2.1, and the recirculation zone is defined subsequently.

4.2.1 Gas-particle corner flow model

The gas-particle corner flow model at the corner is formulated by one-way coupled E-L scheme, in which the flow pattern at the corner is formulated via incompressible laminar flow assumption and the particle dynamics is investigated by Newtown's second law.

The governing equation for a 2-D incompressible corner flow is described by Naiver Stokes equation

$$\rho_f \frac{\partial \mathbf{V}}{\partial t} + \rho_f (\mathbf{V} \cdot \nabla) \mathbf{V} = \rho_f \mathbf{f} - \nabla p + \mu \nabla^2 \mathbf{V} \quad (4.1)$$

where $\mathbf{V} = (u, v)$ is the fluid velocity, ρ_f the fluid density, μ the dynamic viscosity, ∇p the pressure gradient, $\nabla = (\partial/\partial x, \partial/\partial y)$ the Hamilton operator, and $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$ the Laplace operator. The velocity inlet and outlet are set at the entrance of the corner flow and the border of the computational domain, respectively. The non-slip boundary condition at the walls of the corner flow is given by

$$\begin{aligned} u &= 0 & \text{at } y &= 0 \\ v &= 0 & \text{at } x &= 0 \end{aligned} \quad (4.2)$$

The motion of a small particle (particle diameter $d_p \leq 1 \mu m$) is determined by the net force in the flow field. The particles inside the fluid field are mainly

subjected to the following forces, friction $\mathbf{F}_f$ caused by relative velocity, the pressure gradient force $\mathbf{F}_p$, gravity $\mathbf{F}_g$, buoyancy $\mathbf{F}_b$, Van de Waals force $\mathbf{F}_{LvdW}$ if the particle is very close to the wall, Saffman lift force $\mathbf{F}_{sl}$ and Magnus force $\mathbf{F}_m$ due to the particle rotation [9]. Therefore, the resultant force $\mathbf{F}$ is expressed as

$$\mathbf{F} = \mathbf{F}_p + \mathbf{F}_f + \mathbf{F}_g + \mathbf{F}_b + \mathbf{F}_{sl} + \mathbf{F}_m + \mathbf{F}_{LvdW} \quad (4.3)$$

where $\mathbf{F}_p = -(\pi d_p^3/6)\nabla p$, $\mathbf{F}_f = 3\pi\mu d_p \mathbf{u}_r$ and $\mathbf{F}_g + \mathbf{F}_b = (\rho_p - \rho_f)(\pi d_p^3/6)\mathbf{g}$. $\mathbf{u}_r = \mathbf{V} - \mathbf{V}_p$ is the relative velocity between fluid and particle. The other forces are explained as follows.

Particle rotation generates Saffman lift force, given by the empirical Equation (4.4) proposed by Mei [85], if Reynolds number less than 40, and Magnus lift force, given by Equation (4.5).

$$\begin{aligned} \mathbf{F}_{sl} = & 1.61d_p^2\rho_f\sqrt{\nu}|\nabla\times\mathbf{u}_r|^{-\frac{1}{2}}[\mathbf{u}_r\times(\nabla\times\mathbf{u})][(1-0.3314\beta^{1/2})\exp(-\frac{d_p|\mathbf{u}_r|}{10\nu}) \\ & + 0.3314\beta^{1/2}] \end{aligned} \quad (4.4)$$

$$\mathbf{F}_m = \frac{\pi}{8}d_p^3\rho_f[(\frac{1}{2}\nabla\times\mathbf{u} - \omega_d)\times\mathbf{u}_r] \quad (4.5)$$

where ω_d is the angular velocity of the particle, $\beta = (d_p/2|\mathbf{u}_r|)|\nabla\times\mathbf{u}|$, and $\nabla\times\bullet$ represents the curl of a vector.

In addition, particles are influenced by London-Van der Waals(LvdW) F_{LvdW} to remain attached on the wall, if they are close to the wall surfaces. F_{LvdW} may be approximately formulated by neglecting the repulsive effect through Lifschitz approach, if the dispersion between the molecular is dominated [169], given by

$$F_{LvdW} = \frac{h\nu d_p}{16\pi d^2} \quad (4.6)$$

where d is the vertical distance between particle and wall surface, h the Planck's constant, and ν the frequency. $E_L = h\nu$ ranges from 0.6 to 9.0 eV by different material properties [169].

In order to evaluate the particle movement, the residual particle concentration C_{ip} at time t is defined as

$$C_{ip} = \frac{1}{t_s - t} \int_t^{t_s} \frac{N_{ip}}{O_c} dt \quad (4.7)$$

where N_{ip} is the number of particles inside the corner zone, $t_s - t$ the smooth duration and O_c the evaluation area.

4.2.2 Definition of recirculation zone

As shown in Figure 4.1(b), the gas-particle corner flow area is divided into three self-defined zones, recirculation, direct flow and ambient flow zones. Particles in the direct flow zone are transported out of the corner area quickly, and those in the ambient flow zones drift away due to the weak flow. However, the particles in the recirculation zone are trapped inside, in which one or more vortices exist

in the recirculation zone, leading to the flow recycled itself in this zone and thus resulting in a higher particle concentration at the corner. Regarding an incompressible corner flow, the larger recirculation zone indicates more fluidic particles involved in it. Therefore, a variant recirculation zone continuously releases or absorbs fluidic particles, and correspondingly decreases or increases the possibility of solid particles trapped into the zone. Hence, the local particle concentration at the corner area is controllable by the variation of profile of the recirculation zone.

Based on the minimum mass flux principle, the recirculation zone is defined mathematically as a set of 2D simply connected zones z varied over time t enclosed by a continuous line L_c that distinguishes the recirculation zone from the direct flow zone, and the two segments intersected between L_c and coordinate axes. At the boundary of the recirculation zone L_c , the net mass flux is supposed to be minimum, expressed as

$$J = \min(\Delta Q) = \int_{L_c} \rho_f \chi(\mathbf{V} \cdot \mathbf{n}) dl \quad \text{subject to } A \geq A_0 \quad \text{and} \quad \min(A) \quad (4.8)$$

where $\mathbf{n}$ is the unit normal vector of L_c , $\chi(\cdot)$ the step function A the area of the recirculation zone and A_0 a threshold value of A in case of unreasonable small value. The second constraint condition, namely $\min(A)$, requires a minimum recirculation zone among all the L_c satisfying the minimum mass flux principle, and it avoids L_c being over-defined into the direct flow zone. It is noted that $L_c \in \mathbb{Z}$ are solved independently at different time t_i , represented by

$\mathbb{Z} = \{L_c^{t_1}, L_c^{t_2}, \dots, L_c^{t_i}, \dots, L_c^{t_f}\}$. The profiles of the recirculation zone $\mathbb{Z}$ are further concluded as a discrete temporal characteristic, namely the area $A[k]$ of the recirculation zone at each sampling instant k . The new information set $\mathbb{R} = \{A[k], \dots, A[k+n]\}$ contains size information of the recirculation zone. Although the elements in $\mathbb{R}$ are determined independently at different time t_i , they still have a non-linear relationship with each other due to the continuity of the fluid field.

4.3 Development of NN-MPC controller

In this capture, a neural network based model predictive controller is developed to control the profile of the recirculation zone $\mathbb{R}$, in order to control the local particle concentration at the corner. The schematic flow chart of NN-MPC to optimize residual particle concentration in a gas-particle corner flow is shown in Figure 4.2. In Section 4.3.1, the non-linear characteristic of the transient profile, namely the area of the recirculation zone, is learned by a NN model. The NN-MPC algorithm is subsequently developed in Section 4.3.2.

Figure 4.2 Schematic flow chart of NN-MPC to optimize residual particle concentration in a gas-particle corner flow

4.3.1 NN leaning of recirculation zone characteristics

Based on the published investigation on corner flow in potential assumption [80], it is noted that the fluidic particles in a potential corner flow are influenced by mirrored-point- vortices. The trajectory of point vortex center moves chaotically inside the corner and can be controlled by the amplitude of inlet flow [78]. Similarly, the recirculation zone in laminar flow may be also controllable by the intensity of inlet flow, in which several vortices are involved in this zone and change the particle movement inside it. The increase/decrease of the recirculation zone size absorbs/excludes fluidic particle and conveys to solid particle inwards/outwards the recirculation zone. Therefore, the variation of recirculation zone size controlled by the inlet flow intensity may be implemented to change the solid particle concentration at the corner. However, it is very difficult to describe this relationship between the time-variant inlet flow intensity $e[k]$ and area of the recirculation zone $A[k]$ theoretically. In this work, the non-linear relationship is learned by a radial basis function neural network (RBF-NN), of which the structure of a P-input and single-output RBF-NN is depicted in Figure 4.2 and formulated by

$$A[k] = NN(e[k]) = w_0 + \sum_{p=1}^P \sum_{q=1}^Q w_p^o \mathbf{g}(-\|w_{pq}^i I_p(e[k]) - c_q\|^2) \quad (4.9)$$

where P and Q are the numbers of input and hidden nodes, $\mathbf{g}(\cdot)$ and c_q the active function and the bias of each hidden node, w_{pq}^i and w_p^o the weight matrixes of input layer from p th input node to q th hidden node and output layer from q th hidden node to output layer, respectively. w_0 is the output bias. In this

equation, the number of nodes in input layer $I_p(e[k])$ is related to the order of the model. The RBF-NN is trained by the sufficient number of data to describe the non-linear relationship between the inlet flow intensity $e[k]$ and the area of recirculation zone $A[k]$, and then implemented for controller design.

Figure 4.3 Structure of the RBF-NN with p input nodes, Q hidden nodes and single output node

4.3.2 Design of MPC controller

As well known, controlling a process with strong non-linearity requires high computational ability. Alternatively, a linear approximated process model shows the equivalent closed-loop control performance as the full non-linear optimization, but with much more computational efficiency and a wider selection of control algorithm [138, 173]. In this work, the controller is developed by MPC algorithm based on the linear approximation of the nonlinear NN model to optimize the recirculation area, in order to control the local particle concentration in the gas-particle corner flow. The linearized model of NN is expressed as

$$A(k) = \sum_{m=1}^{n_B} b_m(k)e[k-m] - \sum_{m=1}^{n_A} a_m(k)A[k-m] \quad (4.10)$$

where a_m and b_m are coefficients of the linearized model, n_A and n_B the horizons of the input and output, respectively. Equation (4.10) is further written in an increment form as

$$\hat{\mathbf{A}}(k) = \mathbf{G}(k) \Delta \mathbf{e}(k) + \mathbf{A}^0(k) \quad (4.11)$$

where $\hat{\mathbf{A}}(k)$ is the prediction vector of the output and $\Delta \mathbf{e}[k] = \mathbf{e}[k] - \mathbf{e}[k-1]$.

$\mathbf{G}(k)$ indicates the dynamic matrix, given by

$$\mathbf{G}(k) = \begin{bmatrix} s_1(k) & 0 & \cdots & 0 \\ s_2(k) & s_1(k) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ s_N(k) & s_{N-1}(k) & \cdots & s_{N-N_u+1}(k) \end{bmatrix} \quad (4.12)$$

and $s_j(k)$ is determined by

$$s_j(k) = \sum_{i=1}^{\min(j, n_B)} b_i(k) - \sum_{i=1}^{\min(j-1, n_A)} a_i(k) s_{j-i}(k) \quad (4.13)$$

Here, the control algorithm is developed by MPC based on the linearized NN model, namely Equation (4.11), in which the optimization function is given by

$$\begin{aligned} J_{\text{mpc}} &= \min \text{ or } \max \{ \mathbf{A}^T \mathbf{A} + \Delta \mathbf{e}^T \Delta \mathbf{e} \} \\ \text{subject to} \quad & |e[k]| \leq e_m \end{aligned} \quad (4.14)$$

where $\mathbf{e}^T \mathbf{e}$ is equivalent to the energy consumption of the control effort, e_m is the constraint of the control input. Based on the linearized model, namely Equations (4.11) to (4.13), and optimization function, namely Equation (4.14), the NN-MPC is thus solved by the standard quadratic programming [138, 173].

4.4 Validation of the two-phase flow model

The validation of the present two-phase flow model is carried out with the comparison against the theoretical and experimental work by Julien [170, 174]. In the published experimental work, a water-sediment mixture with a concentration of 50 g/L was placed in a 3L beaker, driven by a magnetic stirrer at the bottom. A vortex was generated by the stirring behavior and approximated by a Rankine point vortex model theoretically [170, 174], in which a vortex core rotated as a rigid body at the centre of vortex and induced the surrounding irrotational fluid. Therefore, a rotating cylindrical rigid vortex core is employed in the present validation model, located at the centre of 2D axial symmetry water domain, as shown in Figure 4.4. A total number of 20,000 sediments are released freely at time $t=0s$, and the transient simulation lasts 50s. The London-Van der Waals force is ignored in the validation model due to relatively small amplitude. The model input parameters are consistent with those the theoretical and experimental works by Julien [170, 174], and listed down in Table 4.1.

Table 4.1 Input parameters for two-phase point vortex model for validation[170, 174]

parameters	symbol	value
radius of vortex core	r_0	0.0096 m
length of water domain	r_i	0.09 m
height of water domain	h	0.15 m
angular velocity of vortex core	ω	71 /s
ratio of density	C_p	2.73
diameter of particles	d_p	6.4×10^{-6} m
dynamic viscosity	μ	1×10^{-3} Pa · s

Figure 4.4 Schematic illustration of the two-phase point vortex flow model for validation

Figure 4.5 Streamline and sediment position on rz plane of the two-phase point-vortex model at $t=50s$

The streamline of the fluid and the sediment position on rz plane at $t=50s$ are plotted in Figure 4.5. The sediments are driven by the several vortices in the fluid, resulting in time-varied local concentration in the fluid. However, the point

vortex in the published work [170, 174] is treated as a steady rotating status, in which the sediment concentration is measured without considering the transient behavior. For comparison, the normalized sediment concentration $C_p / C_{p\infty}$ in radial direction r is sampled with an interval of 1s from 30 to 50s in present validation work and plotted by a format of error bar in Figure 4.6(a). The solid line illustrates the average $C_p / C_{p\infty}$ during the period of 30 to 50s, and the maximum and minimum of the error bar indicate the highest and lowest $C_p / C_{p\infty}$ during 30 to 50s. In this figure, the average of $C_p / C_{p\infty}$ has a similar trend with the experimental and theoretical data, namely increasing from the vortex core and then remaining flat, and the error bar of the simulation results covers the experimental data. However, a lower average concentration is found within $r / r_0 \leq 3$ in the simulation than the experiments, since the vortex core is treated as a rigid bar with a non-penetration boundary condition on the wall in current validation, as shown in Figure 4.6. The average concentration increases linearly from the edge of the vortex core and tends to be flat if $r / r_0 > 3$, which is consistent with the experiment measurement. Moreover, the variation of the global error η , defined in Equation (4.15) [175], is evaluated between simulation and experiments with an interval of 1s during 30 to 50s, subject to different ranges of r / r_0 . As plotted in Figure 4.6(b), the global error η decreases significantly in the peripheral area of the point vortex, and reaches the minimum $\eta = 6.591\%$ at 47s if $r / r_0 \geq 3.2$. Thereby, it is claimed that the present model has a satisfactory agreement with theoretical and experimental work for a vortex involved two-phase flow.

$$\eta = \sqrt{\sum_{i=0}^N (C_{pi} - C_{pi}^e)^2 / N} / |C_{pi,max}| \quad (4.15)$$

where C_{pi} is the simulation concentration, C_{pi}^e the measurement from the experiment, N the total number of the data, and $C_{pi,max}$ the maximum of the simulation, respectively.

Figure 4.6 Validation of the two-phase flow model against the experimental and theoretical work by Julien [170, 174] (a) averaged sediment concentration in radial direction from 30 to 50s (b) variation global error between simulation and experiments during 30 to 50s subject to different ranges of r / r_0

4.5 Simulation configuration, results and discussions

The simulation results and discussions are presented in this capture. The computational configuration and simulation results of the gas-particle corner flow with laminar flow assumption are presented in Section 4.4.1. After that, the proposed NN-MPC is employed to a practical scenario in Section 4.4.2, as minimizing the local bioaerosol concentration at an indoor corner with optimal energy consumption.

Table 4.2 Inputs of the two-phase corner flow model

Parameter	Symbol	Value
Diameter of particles	d_p	1 μm [37]
Ratio of density	C_p	1.205×10^{-3} [171]
Kinematic viscosity	ν	$1.68 \times 10^{-5} \text{ m}^2/\text{s}$ [171]
Lifshitz-van der Waals constant	E_L	0.6 eV [168]
Restitution coefficient	e	0.7
Friction coefficient	f	0.3 [172]
Length of corner zone	l_o	1 m

4.5.1 Simulation configuration of gas-particle two phase flow

The simulations by the gas-particle model are conducted by the laminar flow and particle tracing for fluid flow modules in commercial software COMSOL Multiphysics®. As shown in Figure 4.1(b) for the computational domain of the corner area, the ongoing air comes from the ventilation outlet located at $(0, l_o)$, lashes towards the x -axis. 50×50 particles are released at 0s and 5s in a $0.5l_o \times 0.5l_o$ square of the computational domain. The control objective is to achieve minimal residual particle concentration C_{ip} at the corner, which indicates the higher probability of a bioaerosol to be moved out of the corner area. The model input for the particle and geometry of the corner is tabulated in Table 4.2. Moreover, the gas-particle corner flow model is simulated from 0s to 50s with the time interval 0.01s. The time-dependant solve is PARDISO with nested dissection multithreaded pre-ordering algorithm. The maximum number of refinements of iteration is set as 15, and the absolute relative tolerance is $1e-2$ with the tolerance

factor 0.05 for velocity and 1 for pressure. Other settings are kept as default in the software.

Table 4.3 Meshing details of grid convergence study for laminar corner flow

Mesh scheme	Numbers of Element	Min. element quality	Average element quality	Element area ratio
Fine	2215	0.1624	0.8419	8.824e-3
Finer	4632	0.1549	0.8538	1.301e-2
Extra Fine	10979	0.1775	0.8659	5.528e-3

Table 4.4 Grid convergence study for laminar corner flow

Point No.	Convergence order p	Grid convergence index GSI_{12}	Grid convergence index GSI_{23}
$P_1(0.1,0.1)$	1.0724	17.45%	84.67%
$P_2(0.2,0.2)$	1.3517	12.99%	175.07%
$P_3(0.3,0.3)$	1.8688	4.75%	29.47%

The grid convergence study (GCS) of the current CFD work for laminar corner flow is conducted via Richardson extrapolation method [176]. The flow field is computed by three grids with different schemes in COMSOL Multiphysics meshing module, such as “Fine”, “Finer” and “Extra Fine”, as tabulated in 4.3. The velocity magnitudes at 4 representative points are computed in the flow field, namely $P_1(0.1,0.1)$, $P_2(0.2,0.2)$, $P_3(0.3,0.3)$. Based on the Richardson extrapolation methods, the order of convergence $p = \ln[(V_3 - V_2) / (V_2 - V_1)] / \ln 2$, and the grid convergence index

$GSI_{mm} = F_s |(V_m - V_n) / V_m| / (2^p - 1)$ between two neighborhood girding schemes GSI_{12} and GSI_{23} with the safety factor $F_s = 1.25$ are calculated, as tabulated in Table 4.4. The theoretical order of convergence is $p_t = 2$. As shown in Table 4.4, the order of convergence $p_{13} = 1.8688$ is closer to the theoretical value at the point $P_3(0.3, 0.3)$. The reason may be explained by the grid rid stretching, grid quality at the corner point and the influence of turbulence inside recirculation zone. It is also concluded that the estimated velocity field has an error range about 4.75% by the finest meshing at $P_3(0.3, 0.3)$.

4.5.2 Case study I: Particle dynamics without control at corner

Figure 4.7 illustrates the streamline of the corner flow and the evolution of particle movement at some representative time instants. In these figures, it is very clear that most of particles are trapped inside the recirculation zone, while particles in the direct flow zone are transported out of the corner area quickly.

In order to identify the NN model for the characteristics of the recirculation zone, a white-noise is imposed on the corner flow as the velocity input at the top boundary of the computational domain. The input numerically equals the practical ventilation rate and is essential to the energy consumption that is involved in the objective function in Equation (4.14). As shown in Figure 4.8 an input $\bar{e}_c(\tau)$ is randomly generated within a 15% constrained variation of the original ventilation rate $\bar{e}_n(\tau) = 1$, considering the basic requirement of ventilation rate and comfort level for residents. In order to

avoid the turbulence caused by the drastic changes on the input, resulting in uncontrolled process, the input is given delay of 1s at each amplitude.

Figure 4.7 Streamline of corner flow, evolution of particle distribution, and division of the recirculation zone at five representative time instants (a) $t=4s$, (b) $t=14s$, (c) $t=24s$, (d) $t=34s$, (e) $t=44s$.

Figure 4.8 White-noise input for identification of the NN model

According to Equation (4.7), the recirculation zone is defined as a time-varied area enclosed at the corner, by the curved L_c and two segments of axes. It is found that the net flux on the central of L_c dominates much more than that near the intersections with axes. For simplification, a straight line L_c is considered approximately to separate the recirculation zone from direct flow one to form a triangular recirculation zone, and then it is determined by the grid search technique through minimum net flux principle. The divisions of the recirculation zone are depicted by the red solid line in Figure 4.7 at some representative time instants, showing a good agreement with the streamline distinguished the recirculation zone and direct flow zone. The particle distributions at those time instants are also plotted as the black solid spots in Figure 4.7. The variation of the recirculation zone area A with time is smoothed with 0.5s time span, and then plotted in Figure 4.9. $A[k]$ is associated with the control input, which facilitates the controllable absorption and elimination of both fluidic and solid particles, due to the mass conservation of incompressible flow. Figure 4.10 shows the variation of normalized particle concentration with

time and the evaluated areas which are enclosed by part of axes and inclined lines in the PiP. In this figure, the particle concentration drops quickly after released freely due to the direct flow zone. After that, the vortices in the recirculation zone dominates the residual particle concentration at the corner, in which it behaves as a fluctuated curve after 10s in Figure 4.10, due to the variation of recirculation zone size and the adhesion effects from the Van der Waals force. If the area is closer to the corner vertex, the particle concentration remains higher, which indicates that it is much more difficult to remove the particles activating closer to the corner vertex out of the corner zone, if a continuous inlet flow is necessary, such as the basic requirement of ventilation.

Figure 4.9 Variation of recirculation zone area $A[k]$ with sampling instant k

Figure 4.10 Variation of normalized particle concentration inside three different lines

4.5.3 Case study II: Minimization of residual bioaerosol concentration at the corner with optimized energy consumption via NN-MPC controller

The nonlinear relationship between the varied recirculation zone area and the intensity of inlet flow is trained with a NN model with a single hidden layer RBF-NN structure, with 100 hidden nodes and five order delay on input, namely $\bar{e}_c(\tau)$, and 20 order for model output, namely the area of the recirculation area A_s . Except the beginning 4s to form a steady flow pattern at the corner, 4590 groups of data are collected from simulation, 70% of which are used to trained NN model and 15% are used to validate and test the NN model, respectively. As illustrated in Figure 4.11, Both of the trained NN model and the linearized NN model have great accordance with the original data since the maximum of relative error are smaller than 1.5%. The root-mean-square error (RMSE), given in Equation (4.16), is 5.3×10^{-4} between the NN model and values from gas-particle corner flow simulation, and 1.7×10^{-3} between linearized NN model and the simulated value.

$$RMSE = \sqrt{\sum_{k=1}^{k=N} (\hat{y}_k - y_k)^2 / N} \quad (4.16)$$

where $\hat{y}_k$ and y_k represent the predicted and simulated value. N is the total number of sampling instants.

By solving the standard quadratic programming based on Equations (4.11) to (4.14), the time-varied control input by NN-MPC controller is illustrated in Figure 4.12. The control input is then imposed on the gas-particle corner flow model. As shown in Figure 4.13, the particle concentrations at the corner are significantly reduced after imposed NN-MPC control algorithm than a natural control (zero-control) condition. The average of particle concentrations by NN-MPC and natural control, and their relative errors are detailed in Table 4.5, in which the relative errors indicate the probability of bioaerosols removed out of corner zone. For example, if the is imposed, the probability of bioaerosols staying in the corner area, enclosed by axes and Line 2, is reduced by 25.42% via proposed NN-MPC control than that via natural ventilation. It is thus concluded that the proposed NN-MPC algorithm is effective to control the discrete-phase concentration in a gas-particle laminar corner flow with optimized energy consumption, via optimization of the area of vortex-involved circulation zone.

Figure 4.11 Comparisons of predicted recirculation zone area (a), and corresponding relative simulation error (b) compared with NN and linearized NN models

Figure 4.12 Control input by NN-MPC algorithm

Figure 4.13 Comparison of particle concentration in different corner areas between natural ventilation (no control) and NN-MPC control

Table 4.5 Average of particle concentrations in different areas by imposing natural condition and NN-MPC control input

	Area (m^2)	Natural ($/\text{m}^2$)	NN-MPC ($/\text{m}^2$)	Relative error (%)
Line 1	0.125	7411	7163	7.56
Line 2	0.18	6587	5132	25.42
Line 3	0.245	5133	3899	27.52

4.6 Remarks

The improvement of local bioaerosol concentration is realized by control of the forced corner flow with optimal energy efficiency at an indoor environment. The feature of the vortex involved corner flow is parameterized by the area of recirculation zone based on the minimum net flux principle. The control strategy is then developed by the trained NN method to learn a time-varied recirculation zone and NN-MPC based algorithm. The simulation results show that the proposed control strategy is able to decrease the detergent concentration, or

increase the detergent concentration, with optimal energy consumption via setting different objective functions. In addition, the present machine learning based method addresses the difficulty in solving variant parameters of the fluid field and in multi-phase control problem, such as the area of recirculation zone in the present work, which is hardly solved by physical method. Furthermore, the proposed platform broadens the way to address the control of particle concentration in a vortex-involved problem, in which the vortex may be used as a tool to transfer particles to desired area in a fluid field.

Chapter 5 Data-driven control of particle concentration within a turbulent corner flow via proportional-integral-derivative (PID) controller with optimized energy consumption

In this chapter, a PID control is proposed to optimize the bioaerosol concentration at an indoor corner via a gas-particle turbulent corner flow model with energy efficiency. The description of the problem is stated in Section 5.1, followed by development of the gas-particle turbulent corner flow model, in which the turbulent effect is simulated by Menter's Shear Stress Transport (SST) $k - \omega$ model, and the particle phase simulated by Eulerian-Lagrangian scheme. In Section 5.4, the present model is valid against experimental and simulation results from open literature. After that, the model is configured to solve the issue of bioaerosol pollution at an indoor corner. Two case studies are then simulated in order to design a PID controller to minimize the residual bioaerosol concentration with optimized energy consumption for control actuation. Finally, several remarks are discussed in Section 5.6.

5.1 Problem statement

The schematic of the present indoor corner flow is shown in Figure 5.1(a), defined as the area around the intersection between wall and ceiling. The airflow is transported from the ventilation duct through the outlet to the corner area. As shown in Figure 5.1(a), a conceptional control actuator is placed near the outlet to modulate cross sectional area of the duct, resulting in small variation of the flowrate. In addition, the corner flow may be simplified as a 2D flow due to the infinite length in horizontal direction, namely z -axis. As shown in Figure 5.1(b), the computational domain for corner is defined by a square located at original

point $O(0, 0)$, and the inlet airflow is ventilated into the corner area through the outlet located at the right-top border of the domain. Moreover, the particles, are initially suspended in the self-defined triangle area, and then driven by the airflow. Apart from that, the characteristic length of the corner structure is defined as the length of the corner domain $l_0 = 1 \text{ m}$, such that Reynolds number $Re \approx 66000$. Therefore, it is necessary to consider the turbulent effect on the corner flow.

Figure 5.1 Schematics of (a) the indoor corner with bioaerosol pollution, and (b) computation domain of the two-phase turbulent corner flow model

5.2 Modelling of gas-particle turbulent corner flow

In this section, the gas-particle turbulent corner flow is developed for simulation of bioaerosol movement at an indoor corner. The gas phase, namely airflow in Section 5.2.1, is simulated by SST $k - \omega$ turbulent model, while the particle phase, namely bioaerosols, traced by Eulerian-Lagrangian scheme in Section 5.2.2.

5.2.1 Dynamics of turbulent gas phase

Theoretically, several assumptions for the gas phase are made as follows: (1) the continuum assumption is stratified to the gas phase since it works at room temperature; (2) incompressible flow is assumed, since air is considered as a Newtonian fluid and with Mach numbers below 0.3. and (3) thermal effect on airflow is neglected.

Based on above assumptions. The gas phase in turbulent corner flow is modelled by Reynolds averaging the Navier-Stokes equation (RANS) and continuity equation, given by

$$\rho_f \frac{\partial \bar{\mathbf{u}}}{\partial t} + \rho_f (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = -\nabla \bar{p} + (\mu + \mu_T) \nabla^2 \bar{\mathbf{u}} \quad (5.1)$$

$$\nabla \cdot \bar{\mathbf{u}} = 0 \quad (5.2)$$

where $\bar{\mathbf{u}} = (u, v)$ is the fluid velocity by statistical average, $\bar{p}$ the fluid pressure by statistical average, ρ_f the fluid density, μ the dynamic viscosity and μ_T turbulent viscosity, respectively.

Here, the SST $k - \omega$ model is used to evaluate the turbulent energy and dissipation, owing to better predictive accuracy for the flow with strong adverse pressure gradient and separation [177-179]. The governing model equations are expressed in terms of the turbulent energy k and specific dissipation ω , presented below without depth discussion.

$$\rho_f \frac{\partial k}{\partial t} + \rho_f \bar{\mathbf{V}} \cdot \nabla k = P - \rho_f \beta_0^* k \omega + \nabla \cdot ((\mu + \sigma_k \mu_T) \nabla k) \quad (5.3)$$

$$\rho_f \frac{\partial \omega}{\partial t} + \rho \bar{\mathbf{V}} \cdot \nabla \omega = \frac{\rho_f \lambda}{\mu_T} P - \rho_f \beta \omega^2 + \nabla \cdot ((\mu + \sigma_\omega \mu_T) + 2(1 - f_{v1}) \frac{\rho_f \sigma_{\omega 2}}{\omega} \nabla \omega \cdot \mathbf{k}) \quad (5.4)$$

where

$$P = \min(P_k, 10 \rho_f \beta_0^* k \omega) \quad (5.5)$$

with production term P_k

$$P_k = \mu_T \{ \nabla \mathbf{V} : [\nabla \mathbf{V} + (\nabla \mathbf{V})^T] - \frac{2}{3} (\nabla \cdot \mathbf{V})^2 \} - \frac{2}{3} \rho_f k \nabla \cdot \mathbf{V} \quad (5.6)$$

where $\cdot : \cdot$ represents a contraction between two tensors. The turbulent viscosity

μ_T is given by

$$\mu_T = \frac{\rho_f a_1 k}{\max(a_1 \omega, S f_{v2})} \quad (5.7)$$

where $S = \sqrt{2 S_{ij} S_{ij}}$ is the characteristic magnitude of mean velocity gradients.

$$\mu_T = \frac{\rho_f a_1 k}{\max(a_1 \omega, S f_{v2})} \quad (5.8)$$

The model constants are defined through interpolation of appropriate inner and outer values,

$$\phi = f_{v1} \phi_1 + (1 - f_{v1}) \phi_2 \text{ for } \phi = \beta, \gamma, \sigma_k, \sigma_\omega \quad (5.9)$$

The interpolation functions f_{v1} and f_{v2} are defined as,

$$\begin{aligned}
f_{v1} &= \tanh(\theta_1^4) \\
\theta_1 &= \min \left[\max \left(\frac{\sqrt{k}}{\beta_0^* \omega l_w}, \frac{500\mu}{\rho \omega l_w^2} \right), \frac{4\rho \sigma_{\omega 2} k}{CD_{k\omega} l_w^2} \right] \\
CD_{k\omega} &= \max \left(\frac{2\rho \sigma_{\omega 2}}{\omega} \nabla \omega \cdot \nabla k, 10^{-10} \right)
\end{aligned} \tag{5.10}$$

where l_w is the distance to the closest wall. l_w is associated with a reference parameter l_{ref} in SST model, where the distance between objects and wall are reduced than the actual value. The default model constants are tabulated in Table 5.1.

A no slip condition is applied here, given by

$$\mathbf{u} = 0 \quad k = 0 \quad \lim_{l_w \rightarrow 0} \omega = \frac{6\mu}{\rho \beta_1 l_w^2} \tag{5.11}$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Accurate solutions in the near-wall region require that,

$$l_w^+ = \frac{\rho u_\tau l_w}{\mu} \sim 1 \tag{5.12}$$

where $u_\tau = \sqrt{\tau_w / \rho}$ is the friction velocity which is calculated from the wall shear-stress τ_w . l_w^+ should be about 0.5 for maintaining the convergence rate. Crude approximations for k , ε , ω and ζ can be obtained from the following formulas

$$k = \frac{3}{2} (|\mathbf{U}| I_T)^2 \quad \varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{L_T} \quad \omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4} L_T} \quad \zeta = \frac{2}{3} \tag{5.13}$$

where I_T is the turbulent intensity and $L_T = 0.09L$ is the turbulence length scale referring a plane jet, and L is the jet half width.

Table 5.1 Parameters of SST turbulent model

Parameters	Value	Parameters	Value
β_1	0.075	a_1	0.31
β_2	0.0828	σ_{k1}	0.85
β_0^*	0.09	σ_{k2}	1.0
γ_1	5/9	$\sigma_{\omega 1}$	0.5
r_2	0.44	$\sigma_{\omega 2}$	0.856

5.2.2 Dynamics of bioaerosols

The bioaerosol in the present two-phase turbulent flow model is treated as spherical solid particle. Several assumptions are made for simulation of particle movement at corner, and detailed as follows: (1) the particles are one-way coupled with gas phase, (2) no collision between particles is considered due to low particle loading in real situation, (3) elastic collision is considered between particles and wall, and (4) particles are treated as mass point with angular velocity.

Based on Newton's Second Law, the motion of small particles with the mass m_p and diameter such as $d_p = 1 \mu\text{m}$ is determined by the net force $\mathbf{F}_{\text{net}}$ in the flow field. The particles in the fluid field are mainly subjected to the following forces, the drag force $\mathbf{F}_d$, Saffman's lift force $\mathbf{F}_{sl}$, pressure gradient force $\mathbf{F}_p$, buoyancy $\mathbf{F}_b$, gravity $\mathbf{F}_g$, and Van der Waals $\mathbf{F}_{LvdW}$, if the particles are close to wall. The net force $\mathbf{F}_{\text{net}}$ is then given by

$$\mathbf{F}_{\text{net}} = \mathbf{F}_f + \mathbf{F}_{sl} + \mathbf{F}_p + \mathbf{F}_b + \mathbf{F}_g + \mathbf{F}_{\text{LvdW}} \quad (5.14)$$

where $\mathbf{F}_p = -(\pi d_p^3/6)\nabla p$, and $\mathbf{F}_g + \mathbf{F}_b = (\rho_p - \rho_f)(\pi d_p^3/6)\mathbf{g}$. The other forces are explained as follows.

The drag force $\mathbf{F}_f$ is given by the Schiller-Naumann expression,

$$\mathbf{F}_f = \frac{C_D}{24} \frac{\rho_f d_p |\mathbf{u}_p - \mathbf{u}|}{\mu} \quad (5.15)$$

where $\mathbf{u}_p$ is the particle velocity and C_D the drag coefficient by [180], expressed as

$$C_D = \begin{cases} 24(1 + 0.5 \text{Re}^{0.687})/\text{Re} & \text{Re} \leq 1000 \\ 0.44 & \text{Re} > 1000 \end{cases} \quad (5.16)$$

The turbulent dispersion of the particles is modelled by discrete random walk (DRW) [91], where an instantaneous perturbation is added to the drag force given by the mean velocity field of the fluid, as shown in Equation 5.15. The velocity perturbation Δu is determined by the local turbulent kinetic energy k , and resulted stochastically from uncorrelated Gaussian random numbers ξ with unit variance as follows

$$\mathbf{V}' = \mathbf{V} + \Delta \mathbf{V}, \quad \Delta \mathbf{V} = \xi \sqrt{\frac{2}{3}k} \quad (5.17)$$

The Saffman lift force is given by

$$\begin{aligned} \mathbf{F}_{sl} = & 1.61d_p^2\rho_f\sqrt{\nu}|\nabla\times\mathbf{u}_r|^{-\frac{1}{2}}[\mathbf{u}_r\times(\nabla\times\mathbf{u})][(1-0.3314\beta^{1/2})\exp(-\frac{d_p|\mathbf{u}_r|}{10\nu}) \\ & + 0.3314\beta^{1/2}] \end{aligned} \quad (5.18)$$

In addition, particles are attracted by London-Van der Waals (LvdW) $\mathbf{F}_{LvdW}$, if they are close to the wall, approximately formulated by [169],

$$\mathbf{F}_{LvdW} = \frac{h\nu d_p}{16\pi d^2} \quad (5.19)$$

where d is the distance between particle and wall, h the Planck's constant, and ν the frequency. $E_L = h\nu$ ranges from 0.6 to 9.0 eV by different materials [169].

5.3 Design of PID controller for gas-particle turbulent corner flow

For control of the particle concentration in the gas-particle turbulent corner flow, it is difficult to use the physical-based flow model with complex turbulence as a control plant directly to design the controller. Therefore, a single-input-single-output (SISO) plant is identified to model the relationship between inlet velocity and particle concentration at corner, by simulation data from the gas-particle turbulent corner flow model, as presented in Section 5.2. Based on the identified plant, a PID controller is then designed and implemented for a simulated closed-loop system to construct open-loop input signals for the physical system, namely the gas-particle turbulent corner flow.

5.3.1 System identification by transfer function models

Transfer function $TF(s)$ models are used to characterize behavior of SISO plant, in which the input signal $x(t)$ and output $y(t)$ is mapped by Laplace transform, given by

$$Y(s) = TF(s)X(s) \quad (5.20)$$

where $Y(s) = L[y(t)]$, $X(s) = L[x(t)]$, and $L(\cdot)$ represents the Laplace transform, defined by

$$F(s) = L[f(t)] = \int_0^{\infty} f(t)e^{-st} dt \quad (5.21)$$

The transfer function $TF(s)$ is a ratio of polynomials, where the order of the denominator polynomial (number of poles) determines the order of the model. The polynomial coefficients are the free parameters of the transfer function structure, which are identified to fit the measurements of the gas-particle turbulent corner flow.

Figure 5.2 Diagram of a feedback system containing a controller and an identified plant model

For SISO plant to appropriately capture the dynamics of the gas-particle turbulent corner flow, the responses are acquired by three excitation signals,

namely step, chirp and white noise signals. Step response is one of the most commonly used excitation signals for linearized system. Apart from that, a white noise with random amplitude and chirp signals with time-varied frequency are excited to the two-phase turbulent corner flow respectively, in order to capture the system dynamics. The corresponding SISO plants are then identified by fitting the input data, namely inlet flow rate, and output data, namely residual particle concentration.

5.3.2 PID controller design by the reduced model

As well known, the rate and timing of bioaerosol releasing are determined by the biological and environmental characteristics, such as nourishing level, species, temperature, and airflow rate [164, 165]. Furthermore, it is difficult to predict and detect the timing and location of released bioaerosols [164]. Therefore, the intensively and continuously releasing particle bioaerosols are simulated, instead of an individual randomly released bioaerosol. As a result, the control of residual concentration for bioaerosols is equivalent to the control of probability of bioaerosol staying in corner area. For example, if the single bioaerosol is released into the corner zone, it is removed out with a larger probability, if the residual concentration decreases in the intensively released simulation.

Figure 5.3 Schematic flow chart of controller design to optimize residual particle concentration in a gas-particle turbulent corner flow

Schematic flow chart of controller design to optimize residual particle concentration in a gas-particle turbulent corner flow is illustrated in Figure 5.3. After the SISO plant is identified through the excitation signal as input data and corresponding residual particle concentration as the output data, a controller is designed in a closed-loop system with a set point, defined as the desire residual particle concentration. The signal processed by the controller is then implemented as an open-loop control input signal to inlet flow rate, acting on the gas-particle turbulent corner flow. The control performances by different controllers are compared finally with the consideration of the optimized energy consumption.

As a classic controller, the PID controller in a closed loop system is designed outputs a signal $u(t)$ with the purpose to achieve a desired plant output $y(t)$ that corresponds to a set-point signal r . This is done by applying different gains to proportional, integrative and derivative terms of the error signal $e(t) = r(t) - y(t)$

$$x(t) = k_p e(t) + k_i \int_0^t e(\tau) d\tau + k_d \frac{de(t)}{dt} \quad (5.22)$$

where P , I , and D are parameters that can be tuned to suit desired specifications. For a more general formulation of PID controller, a N filter coefficient is considered in derivative item. Therefore, the transfer function of a PID controller after Laplace transformation is given by

$$C_{\text{PID}}(s) = P + \frac{I}{s} + D \frac{N}{1 + N \frac{1}{s}} \quad (5.23)$$

The amplitude of the control signal may be limited by the physical processes, such as constraints on the velocity coming out of a ventilation outlet. The control signal is called saturated if it reaches the physical limit.

5.4 Validation of two-phase flow model with backward facing step experiment

For validation of the two-phase flow model against published experimental and simulation results, the uniform inlet velocity is set along the inlet. The fluid is then simulated along a long inlet channel to form a fully developed profile before reaching the step.

The present two-phase turbulent model is implemented in laminar flow and particle tracing for fluid flow modules in COMSOL Multiphysics 5.4©, where default model settings and constants of the software are used in general if not specified. The identification is built in MATLAB routines, and control loops are implemented via SIMULINK.

For validation of the present gas-particle turbulent corner flow model, BFS is a suitable structure for comparison, since it contains flow separation and time-varied recirculation zones at corner located behind the step, where they have

similar presence and importance in the present study. The model is validated against experimental [92] and simulation works [90] of a particle laden flow over a backward-facing step, in which velocity profiles and maximum negative velocities at downstream of the step are compared with experiments.

Table 5.2 Parameters for validation against experiment.

Property	Value
Step height h_0	0.025 m
Inlet length	1.254 m
Inlet height	0.025m
Outlet length	0.8 m
Dynamic viscosity	1.825×10^{-5} kg/ms
Fluid density	1.204kg/m ³
Free stream velocity	39.67 m/s
Particle density	810 kg/m ³
Particle diameter	1 μ m

The schematic of the BFS is presented in Figure 5.4, with $(x, y) = (0, 0)$ at beginning and bottom of the step. The positive x -axis is along the stream-wise direction to the left and positive y -axis upwards. Dimensions as well as fluid and particle properties are compiled in Table 5.1. A sufficiently long inlet length is taken to ensure fully developed flow at the step, giving a normal inflow velocity of 35.5 m/s at the inlet. No slip boundary condition is set on the walls and 0 pressure at the outlet. The fluid phase is converged to a stationary solution, as

shown in Figure 5.5 for velocity contour around the step. The free-stream velocity u_0 is found to be 39.67 m/s at $12h_0$ upstream the step, producing a Reynolds number around 64000. 5000 particles with are released at $12h_0$ downstream the step, with initial velocities identical to that of the fluid phase. The trajectories are computed using Lagrangian particle tracking with drag force, lift, pressure gradient and gravity forces composed on the particles.

The validation errors are calculated by taking the root mean square error between simulated and experimental values, relative to the largest simulated value, given by

$$e_{global} = \frac{\sqrt{\frac{1}{N} \sum (v_s - v_e)^2}}{\max(v_s)} \quad (5.24)$$

where e_{global} is the global error, v_s the simulation results, v_e the experimental measurements, and N is the total number of the compared points, respectively.

Particle velocity profiles in stream-wise direction are shown in Figure 5.6, compared to experimental work by Ruck and Makiola [92] and simulation work by Tian *et al.* [90]. The measured particle profiles are 9th order polynomials fit to the data, with best fit based on minimized root mean square error (RMSE). The global relative errors compared to Ruck and Makiola [92] for each profile from left to right are 5.24%, 9.19% and 8.29%.

Figure 5.4 Geometry of the backward facing step, with step height of 0.025 m, the inlet and outlet lengths of 1.25 m and 0.87m, respectively.

Figure 5.5 Velocity contour with streamlines around the backward facing step.

Figure 5.6 Comparison of particle velocity profiles from the present simulations with the experimental [92] and simulation (realizable $k-\varepsilon$) [90] studies

As shown in Figure 5.7, the maximum negative velocities of the particles downstream the step is observed. The maximum velocity values are taken in intervals of size 10^{-4} m for $x = (0, 0.3)$. A 6-order polynomial is fit to the particle data based on minimized RMSE. The global relative error compared to experiment is calculated by Equation 5.24 as 12.2%.

Figure 5.7 Comparison of the maximum negative particle velocity in recirculation zone behind step against the simulation and experimental results

The errors for particle profiles and maximum negative velocity are satisfactory. It is thus proved that the SST $k-\omega$ model is able to produce simulation results with a satisfactory agreement against experiment. The most important aspect of the validation is however to show that the model is able to produce the relevant recirculation phenomena, which is important working medium for control of discrete concentration in a two-phase flow.

5.5 Simulation configuration, results and discussions

In this section, the simulation configuration is present first in Section 5.5.1. After that, two case studies are conducted subject to two academic investigations, detailed by Suspending particle dynamics without control at corner in Section 5.5.2, and Control of residual particle concentration at indoor corner with optimized energy consumption via PID controller in Section 5.5.3.

Table 5.3 Parameter configuration for simulations

Property	Value
Inlet height	0.1 m
Inlet length	0.2 m
Wall length	1 m
Roof length	1 m
Side of measurement triangle	0.5 m
Side of release grid	0.15 m
Dynamic viscosity	1.825×10^{-5} kg/ms
Fluid density	1.204 kg/m^3
Particle density	810 kg/m^3
Particle diameter	$1 \mu\text{m}$

5.5.1 Simulation configuration

The corner flow experiment is set up with geometrical dimensions and fluid and particle properties as given in Table 5.3, based on the geometry in Figure 5.2, with the original point $(x, y) = (0, 0)$ in the bottom left corner. For all the results under this section a constant inlet velocity $v_{in} = 1 \text{ m/s}$ is used for the entire simulation and 1600 particles are released. The present gas-particle turbulent corner flow is simulated in twenty-five continuous seconding with a time step of 0.05 s. The time-dependant solve is PARDISO with automatic pre-ordering algorithm. The maximum number of refinements of iteration is set as 15, and the absolute relative tolerance is $1e-2$ with the tolerance factor 0.05 for all the variables. Other settings are kept as default in the software.

Furthermore, particles are released with zero initial velocity into the corner, in a uniform square grid, such that the particles are released from positions within the zone of recirculation.

Richardson extrapolation method is used for the GSC of the current CFD work for turbulent two-phase corner flow [176]. Three different grids are meshed for GSC and simulated by COMSOL Multiphysics meshing module, as shown by “Normal”, “Extra Fine” and “Extreme Fine” in Table 5.4. Since the velocity around the corner point is essential to the particle movement in current study, the velocities at 3 points around the corner, $P_1(0.9,0.9)$, $P_2(0.8,0.8)$, $P_3(0.7,0.7)$, are supervised for GSC. The safety factor is set up with $F_s = 1.25$ for a three meshing comparison and the theoretical order of convergence is $p_t = 2$. The order of convergence and the grid convergence index between two neighborhood girding schemes are then computed via Richardson extrapolation method, as shown in Table 5.5. The order of convergences of the three points are close to theoretical order in which the point $P_1(0.9,0.9)$ has the closed value as $p = 1.811$. The error range of the estimated velocity field is about 1.64% by the finest meshing at $P_2(0.8,0.8)$. The grid rid stretching, grid quality and the turbulence may be the reason leading to the error of velocity field.

Table 5.4 Meshing details for grid convergence study

Mesh scheme	Numbers of Element	Min. element quality	Average element quality	Element area ratio
Normal	17198	0.1420	0.8431	1.133e-3
Extra fine	18974	0.1396	0.8490	1.827e-3
Extreme fine	33450	0.1467	0.8845	1.278e-2

Table 5.5 Grid convergence study for turbulent corner flow

Point No.	Convergence order p	Grid convergence index GSI_{12}	Grid convergence index GSI_{23}
$P_1(0.9,0.9)$	1.8110	11.66%	28.05%
$P_2(0.8,0.8)$	1.5334	1.64%	2.56%
$P_3(0.7,0.7)$	1.6365	4.45%	8.21%

5.5.2 Case study I: Suspending particle dynamics without control at corner

The simulation is carried out first subject to a case study of suspending particle dynamics without control at corner, in order investigate the dynamics of both fluid and particle phases. The evolution of corner flow streamlines and particle position at three represented time are plotted in Figure 5.8. It is shown that a larger area of recirculation zone is inhibited in corner and the particles are constrained in corner, with the recirculation zone caused by several vortices. However, total amount of particle is reduced with time, since the time-varied recirculation zone excludes the particles if the particles are conveyed to the interface between the border of recirculation zone and external flow. Therefore, the time-varied recirculation zone is closely associated with the particle concentration at corner. Further studies on control of residual particle concentration could be achieved based on the phenomenon.

(a) $t=15s$

(b) $t=20s$

(c) $t=25s$

Figure 5.8 Evolution of corner flow streamline and particle position at (a) $t=15s$, (b) $t=20s$, and (c) $t=25s$

The cluster and individual particle movements are studied as shown in Figures 5.9 and 5.10. The particle positions and velocity at different times are illustrated in Figure 5.9, in which the particles are distributed in the triangle-like recirculation zone and concentrated by one major and several small vortices at the corner. The trajectories of three neighboring particles are shown in Figure 5.10 from 10 to 25 seconds, in which individual particle trajectory is mainly influenced by vortices in the recirculation zone, as well as the random effects by the turbulence. In Figure 5.10 (a), the particle is captured by the small-scaled vortex without leaving the region before $t = 25$ s. However, another particle

leaves the recirculation zone immediately without being captured by any vortex, as shown in Figure 5.10(b). The other particle in Figure 5.10 (c) is captured by the larger recirculation vortex and stays in the corner until the terminal time.

Figure 5.9 Particle positions and velocities, at four different times for 1600 particles released at $t = 10$ s, simulated with discrete random walk

The contribution of the various particle forces is investigated by averaging the total force magnitudes over all particles in the measurement zone. The averaged force contributions over time are plotted in Figure 5.11. It is found that the drag force F_f dominates the net force F_{net} , followed by lift F_{sl} and gravity F_g . The pressure gradient force F_p is at the level of a much lower order with small influence on the dynamics.

Figure 5.10 Trajectories of neighboring particle releases, simulated with discrete random walk, with initial positions at (0.9, 0.8692), (0.9, 0.8731) and (0.9, 0.8769).

Figure 5.11 Measured and averaged mean force imposed on particles within measurement triangle

For system identification of the relationship between inlet flow rate and the residual particle concentration, three excitation input signals are fed as inlet flow rate into the gas-particle turbulent corner flow, including step of 1.2 m/s, chirp and white noise signals, as shown in Figure 5.12. Particularly, the white noise signal remains two seconds for each amplitude to avoid the severe variation of

the corner flow. The residual particle concentration C_r and residual particle reduction C_d are defined by

$$C_r = \frac{N_r}{N_0} \quad C_d = C_m - C_{re} \quad (5.25)$$

where N_r is the amount of residual particles in the particle measurement area, as shown in Figure 5.2, and $N_0 = 1600$ the initial amount of the released particles. C_m and C_{re} are the residual particle concentrations by nature ventilation (1 m/s) and excitation signals.

The variation of residual particle concentrations with time t in the corner is plotted in Figure 5.13, subject to nature ventilation of 1 m/s, and three excitation input signals. It is illustrated that the residual particle concentration C_r is varied with different input signals for inlet flow rate. The comparison of residual particle reduction C_d is plotted in Figure 5.14, in which higher C_d indicates more particle reduction at corner than the nature ventilation of 1 m/s. It is shown that the time variation of particle reduction ability is associated with the input signals. For example, the particles are removed over 4% by the chirp execution input signal, compared with the natural ventilation. However, the C_r by the white noise signal maintains the same level as the natural ventilation during the fifteen seconds. Therefore, a desired reduction of C_r could be potentially achieved by a well-designed control algorithm.

Figure 5.12 Three excitation input singles for system identification

Figure 5.13 Comparison of residual particle concentration C_r by nature ventilation (1 m/s) and three excitation input signals, namely step of 1.2 m/s, chirp, and white noise

Figure 5.14 Comparison of residual particle reduction C_d by step of 1.2 m/s, chirp, and white noise excitation input signals against natural ventilation (1 m/s)

By the residual particle reduction C_d obtained via the simulations, three transfer function models are identified subject to the three excitation input signals, respectively.

A nine-order transfer function $TF_1(s)$ model with 9 poles and 6 zeros is identified to the step response of the physical system, given a step change in velocity from 1 m/s to 1.2 m/s.

$$TF_1(s) = \frac{(0.1846s^6 + 0.4414s^5 + 0.7256s^4 + 6.972s^3 + 1.676s^2 + 7.102s + 3.122)}{(s^9 + 1.737s^8 + 30.99s^7 + 45.65s^6 + 276.5s^5 + 291.4s^4 + 706.8s^3 + 329.5s^2 + 475.7s + 35.69)} \quad (5.26)$$

A fit of 86.51% to the estimation data is achieved for response of the identified SISO plant, as shown in Figure 5.15(a).

A ten-order transfer function $TF_1(s)$ with ten poles and non-zeros, given by Equation 5.26, is identified by the response of a continuously varied fluctuating signal in frequency, namely chirp signal, in which a fit of 84.63% to the estimation data is reached for response of the identified SISO plant, as shown in Figure 5.15(b).

$$TF_2(s) = \frac{0.1216}{(s^{10} + 1.368s^9 + 11.41s^8 + 14.65s^7 + 39.17s^6 + 39.54s^5 + 47.91s^4 + 32.01s^3 + 20.25s^2 + 5.929s + 1.84)} \quad (5.27)$$

Figure 5.15 Comparison of identified transfer function models excited by different (a) step of 1.2, (b) chirp, and (c) white noise excitation

signals, with the relative residual particle concentration C_d by gas-particle turbulent flow simulations

By a six-order transfer function model with six poles and three zeros, given by Equation 5.16, another SISO plant is identified by the response of a randomly fluctuating signal, namely white noise, in which a fit of 59.47% to the estimation data is achieved for response of the identified SISO plant, as shown in Figure 5.15(c).

$$TF_3(s) = \frac{0.137s^3 - 0.345s^2 + 0.4686s + 0.1073}{s^6 + 0.8203s^5 + 12.73s^4 + 5.128s^3 + 34.73s^2 + 2.004s + 12.24} \quad (5.28)$$

As shown in Figure 5.15 (a), (b) and (c), it is illustrated that the three transfer function based SISO plants follow the general trend of the step response but are not able to capture the small transient oscillatory behavior.

5.5.3 Case study II: Control of residual particle concentration at indoor corner with optimized energy consumption via PID controller

Three different PID controllers are designed and tuned, for each of the identified transfer function plants, given by $TF_1(s)$, $TF_2(s)$, and $TF_3(s)$ respectively. Three set points are given for a desired reduction percentage for residual particle reduction C_d , namely 0.10, 0.125, and 0.15. With the consideration of the real ventilation requirement in a room, the control signal for the inlet flow air is constrained with a range from 0.8 m/s to 1.2 m/s. The PID controllers are then tuned in a closed-loop system, as shown in Figure 5.2 and Figure 5.3. The controller parameters and corresponding step response performance of the three

PID controllers are summarized in Table 5.6, including setpoint (SP), proportional coefficient (P), integral coefficient (I), derivative coefficient (D), filter coefficient (N), rising time (RT), settle time (ST) and overshoot (OS).

For the optimization of energy consumption, the instantaneous energy E_{sig} of the control actuation for the inlet flow rate is defined as

$$E_{sig} = \frac{1}{2}(v_0 - v_{sig})^2 \quad (5.29)$$

where v_{sig} is the instantaneous amplitude of the input signal.

Table 5.6 PID controller parameters and corresponding step response performance

TF	No.	SP	P	I	D	N	RT	ST	OS
$TF_1(s)$	1-1	0.10	2.86	1.31	-33.0	0.09	15.3	53.3	13.7%
$TF_1(s)$	1-2	0.125	2.75	1.16	-34.5	0.08	17.1	56.6	12.1%
$TF_1(s)$	1-3	0.15	5.43	1.01	-69.4	0.08	18.1	53.1	7.35%
$TF_2(s)$	2-1	0.1	12.71	9.48	0	100	17.4	70.6	0.18%
$TF_2(s)$	2-2	0.125	0.82	1.45	0	100	6.04	54.8	5.85%
$TF_2(s)$	2-3	0.15	0.18	1.29	0	100	7.88	42	1.01%
$TF_3(s)$	3-1	0.1	0	2.80	0	100	9.23	57.4	26.8%
$TF_3(s)$	3-2	0.125	23.72	17.57	5.47	108.7	2.09	42.8	16.1%
$TF_3(s)$	3-3	0.15	22.56	16.50	5.19	106.7	2.14	43.3	13%

The signals after the PID controller block, as shown in Figure 5.3, are fed as the open-loop control single for the gas-particle turbulent corner flow. The

residual particle reductions C_d by PID controllers against those by natural ventilation are plotted in Figure 5.16(a) with a setpoint 0.1, in Figure 5.17(a) with a setpoint 0.125, and in Figure 5.18(a) with a setpoint 0.15, respectively. The comparison of the control signals for inlet airflow rate, and corresponding accumulated energy consumption for control actuations are illustrated in Figures 5.16 to 5.18 (b) and (c), respectively.

As shown in Figures 5.16 to 5.18, lower residual particle concentrations are achieved by all the PID controller, with positive values of residual particle reduction C_d . Regarding the PID controllers with the same setpoint, it is found that the residual particle reduction C_d varies within a small range by the PID via different transfer function models, namely TF_1 in Equation 5.26, TF_2 in Equation 5.27, and TF_3 in Equation 5.28. However, the largest reductions C_d are obtained, subject to the PID controllers designed by transfer function model with white noise excitation signals, namely PID3-1, PID 3-2 and PID3-3, as shown in Figures 5.16(a) to 5.18(a). it is noted that the three mentioned PID controllers consume more energy than the other two, but result in a limited improvement on particle reduction. In general, the residual particles concentration reduces with a higher setpoint of C_d . However, C_d are not reached in each case, where a possible reason may be the long settle time of the transfer model, as shown in Table 5.6. It is thus concluded that the designed PID controllers are effective for reduction of particle concertation at the corner, in which the reduction ability is associated with the set point and the energy consumption by controller. Furthermore, the similarity is found among the PID control signals. For example, PID3-1, PID2-2, PID2-3, PID3-2, and PID3-3 have the similar shape of control

signals, starting for the bottom limitation, rising with a slop around 15s till the top limitation and maintaining till end. It is interesting to find that the controller with an earlier rising start generally results in more particle removal. Moreover, the small variation of C_d during the initial few seconds after particle releasing may be caused by the random effects of turbulence.

Table 5.7 Total energy consumption E_t , averaged residual particle reduction C_d , and terminal residual particle reduction C_d by different PID controllers

PID controller	E_t	Averaged C_d	Terminal C_d
PID1-1	4.8607	0.0331	0.0425
PID2-1	2.1870	0.0379	0.0600
PID3-1	5.4929	0.0468	0.0675
PID1-2	5.0680	0.0477	0.0631
PID2-2	5.1367	0.0491	0.0706
PID3-2	6.02	0.0550	0.0769
PID1-3	5.2691	0.0521	0.0700
PID2-3	5.09	0.0538	0.0706
PID3-3	6.02	0.0550	0.0769

In addition, the accumulated energy consumption E_t , averaged and the final residual particle reduction C_d are tabulated by Table 5.7, subject to PID controllers with different setpoints. It is shown that the PID controller by TF_3 consumes more energy than the others to achieve more averaged and terminal particle reduction, while the other two consume similar energy but have the similar particle reduction ability. It is necessary to balance the energy

consumption and the control effectiveness, in which more energy may be consumed by a controller with better ability for reduction of particle concentration.

(a)

(b)

(c)

Figure 5.16 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.1

(a)

(b)

(c)

Figure 5.17 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.125

Figure 5.18 Comparison of (a) residual particle reduction C_d , (b) inlet flow rate, and (c) accumulated energy consumption by different TF-based PID controllers with setpoint 0.15

5.6 Remarks

A gas-particle two-phase model at an indoor corner is developed using Lagrangian-Eulerian approach for CFD simulations. The turbulence is modelled

by SST $k - \omega$ for the fluid phase and discrete random walk is employed to the drag force for the particle phase. The model is validated against experimental values of a backward facing step ($Re = 64000$) and an error between experiment and simulation of 12% is achieved when comparing maximum negative velocities behind the step. The drag force makes the largest contribution to the particle dynamics, followed by lift and gravity. Particle trajectory is constrained in recirculation zone at the corner plus random effects due to turbulence. A large number of particles are thus considered in simulations for averaged values, which is equivalent to the probability of particle removal. Transfer function model plants are identified to reveal the correlation between the input, namely inlet flow rate, and the output, namely particle corner concentration, by three excitation signals. The PID controller are thus designed in a closed-loop system to pursue the reduction of the residual particle concentration at corner. After that, the control inputs are extracted from the closed-loop system to feed as an open-loop control input to the gas-particle turbulent corner flow model. Based the simulation results, it is thus concluded that the PID control is effective on the considered two-phase flow control problem, by successfully reducing the residual particle concentration, in which the PID designed by SISO plant with chirp excitation signal has the best performance. Furthermore, it is also necessary to balance the energy consumption and the control effectiveness, in which more energy may be consumed by a controller with better ability for reduction of particle concentration. Regarding the performance of control algorithm, it is convenient and easy to implement the proposed transfer function based PID design to control the particle concentration at corner with optimized energy consumption. However, other data-driven based modeling remains possibility to

capture and modulate the nonlinearities with further improvement on control performance.

Chapter 6 Conclusions and Recommendations

6.1 Conclusions from present work

The present research work focuses on the data-driven control of discrete-phase concentration in two-phase flow with optimized energy consumption. The vortex-involved two-phase corner flow model is developed first subject to potential flow theory, laminar and turbulent flow schemes, respectively. The data-driven control strategies are then designed for modulation of the flow pattern correspondingly by orthogonal design, NN-MPC and PID controllers with optimized energy consumption of control actuation. The proposed approaches demonstrate the effectiveness and applicability of data-driven modeling and control strategies for the complex two-phase control problem, and consider energy consumption simultaneously as important parameter for optimization. Furthermore, the proposed data-driven modeling and control strategies provide a novel way for two-phase corner flow control problem. Therefore, it is unnecessary to construct the physical-based complex two-phase corner flow model for design of controller, and not to require a lot of computational cost for identification of the model characteristics. In conclusion, three major achievements of this thesis arise from the present research, and they are summarized as follows respectively.

The first achievement of the present research provides the data-driven control for a gas-particle potential corner flow model, in which the control strategy for the inlet flow rate is optimized by analyzing simulation data via orthogonal design method, with consideration of the energy consumption.

- In the proposed control strategy, a gas-particle potential flow model with a chaotic moving vortex is developed to simulate the bioaerosol movement at an indoor corner via the Eulerian-Lagrangian scheme, in which the model is validated well by experimental and simulation results for a gas-particle two-phase flow including a single stationary vortex.
- It is found that the bioaerosols are concentrated by the vortex at corner, and thus difficult to be removed via natural ventilation (zero control). However, the bioaerosol concentration is reduced by the evolution of the vortex via periodic interaction with external flow, in which the vortex trajectory is controlled by the airflow from the ventilation outlet.
- The presented approach, consisting of the two-phase potential flow model with moving vortex and control strategy, provides a novel energy-efficient way to improve the indoor air quality, by controllable airflow pattern from ventilation, instead of using extra air cleaning machine or human force. Energy consumption for control of the airflow rate is optimized in the control strategy.
- It is demonstrated that the bioaerosol concentration at corner is energy-efficiently reduced by a Pulse Width Modulation controller with low amplitude, proper duty factor, period and time delay.

The second achievement is the development of a data-driven control for discrete-phase concentration in the forced laminar corner flow with optimized energy efficiency, in which the control strategy is designed by MPC algorithm, based on a linearized NN model for the correlation between inlet flow rate and the area of recirculation zone.

- In the proposed control strategy, a gas-particle laminar corner flow model is developed to simulate the particle movement at a 90-degree corner via the Eulerian-Lagrangian scheme, in which a circulation zone traps particles around corner. A time-varied circulation zone is further defined mathematically by the minimum net mass flux principle, and determined by grid search technique.
- It is demonstrated that the nonlinear dynamics between the parameterized circulation zone and inlet flow rate is captured well by a NN trained via the simulation data. Based on the linearized NN, an MPC algorithm is implemented to achieve an optimal profile of the recirculation zone with optimal energy consumption.
- The proposed control strategy is employed for reduction of bioaerosol concentration at indoor corner through a flow-rate-controllable air inlet located at ceiling. It is shown from simulations that the bioaerosol concentration is reduced maximumly by 25.42% via the data-driven control (NN-MPC) at indoor corner.

The third achievement is the development of data-driven control of discrete-phase concentration within a gas-particle turbulent corner flow, in which PID controller is designed by transfer function model identified via simulation data, with optimized energy consumption.

- In the proposed control strategy, a gas-particle turbulent corner flow model is developed for simulation of the particle movement through computational fluid dynamics (CFD), in which the turbulent effect is

simulated by SST $k-\varepsilon$ model, and the particle phase simulated by Eulerian-Lagrangian scheme.

- The model is validated against experimental and simulation results of a particle laden flow over a backward facing step, with a satisfactory agreement by a global error of 12.2% for the maximum negative velocity in the recirculation zone.
- It is found that the particle concentration at the corner is reduced after imposing a control signal on inlet flow rate. Therefore, three transfer function models are identified to construct the correlation between inlet flow rate and residual particle concentration, by simulation data from the gas-particle turbulent corner flow model with three excitation input signals. After that, the three PID controllers are designed by closed-loop system to minimize the residual particle concentration at corner, and compared for optimization of energy consumption of control actuation.
- Based on the results, effective controllability is achieved by the three PID controllers, in which the best controller reduces 24.16% of the particle concentration. In addition, the efficient energy consumption is discussed among different sets of controller parameters, based on the requirement of the energy and residual particle concentration.

In conclusion, the entire thesis is constituted by the three achieved contributions mentioned above. It is believed that the present work is meaningful for the development of novel data-driven approaches systematically to control the discrete-phase concentration in a two-phase corner flow, by modulating the flow pattern via the existing vortex in the fluid field, with optimized energy consumption of control actuation. Regarding the different control methods, the

orthogonal design method is obviously easy and convenient to design and apply. However, the “trial-and-error” based algorithm requires plenty work for different simulations. The method is also not intelligent enough, owing to discontinuity of the initial parameter distribution, indicating the determined optimized energy control may be not the optimal. On the other hand, MPC and PID may solve the problem, in which the control inputs are computed by “calculations” instead of “trials”. PID has the advantages for industrial convenience and is easier to design and tune, nevertheless MPC is more applicable for the model with strong nonlinear dynamics and has great controllability with constrained control input and optimized energy consumption. As one of the applications, the proposed approaches are conducted to control the bioaerosol concentration at indoor corner, in order to improve the indoor air quality which is important to the resident health.

6.2 Recommendations for future work

On the basis of the research studies completed in this thesis, several potential topics are recommended for control of discrete-phase concentration for a two-phase flow with optimized energy consumption.

The combination of the potential flow model and laminar/turbulent model may be one of the possible directions based on the current control framework in the future. The schematic flowchart is illustrated in Figure 6.1. The vortex position derived by the analytical model based on potential flow theory will be compared against the one concluded by the laminar flow model. And the difference will be used as an output data while the excitation signals will be treated as an input to train the ML model. After that, the control objective is transferred to manage the vortex position by the compensated from the potential

flow derivation and ML prediction, in order to control the discrete-phase concentration in the two-phase flow. The proposed idea constructs a link between potential flow theory and laminar flow through ML technique.

Figure 6.1 Schematic flowchart for control of discrete-phase concentration by ML technique via comparison between potential flow and laminar flow

It is also interesting to modify the current 2D two-phase flow model to 3D domain, in which the impact may be discussed from the following two aspects.

- a) Extending the computational domain to 3D from 2D coordinate systems not only produces extra turbulence in airflow, but also results in different distributions of particle concentrations. However, both these extra turbulence and different particle-concentration distributions are ignorable in an indoor corner with long horizontal length.
 - In a 3D corner zone, the turbulent velocity field leads to the vorticity and pressure sink in z direction, resulting in a mass flux along the z direction, as shown in the figure below for schematic of 3D corner flow. The mass flux generates more turbulence and influences the size of the recirculation, if it lashes on the side wall of the corner. Additionally, the particles have a relative

velocity in z direction against the flow velocity field, if they drop into the area around vortex centre, resulting in the displacement in z direction. The phenomenon influences the distribution of particle in the 3D corner zone.

Of course, the extension to 3D from 2D scenarios is meaningful and improves the accuracy of the two-phase of corner flow, especially around the dead-end 3D corner. The relevant work will be considered in the future work.

- For achieving the update to 3D from 2D coordinate systems, a 3D corner geometry is required for meshing, and an additional momentum equilibrium equation is added as well, namely the NS equation $\rho_f \partial \mathbf{V} / \partial t + \rho_f (\mathbf{V} \cdot \nabla) \mathbf{V} = \rho_f f - \nabla p + \mu \nabla^2 \mathbf{V}$ in z direction. The force analysis of particles is also necessarily modified in a 3D scenario.

Figure 6.2 Schematic of 3D corner flow.

- b) In terms of control algorithm, both the control medium parameters and control objective in the data-driven control algorithms are necessarily re-designed regarding the changes of two-phase corner flow from 2D to 3D domains. These changes require extra computation, but are comprisable with proper computational skills.

- As an excepted medium parameter, the recirculation zone defined by Equation (4.8) will be enclosed by a 3D curve in the corner space, and modified to the volume of recirculation zone $V(L_{c-3D})$, instead of the area $A(L_{c-2D})$, due to the changes of fluid velocity field from $V(x, y)$ to $V(x, y, z)$. In addition, as an excepted control objective, the residual particle concentration is changed to a 3D variable from $C_p(x, y)$ to $C_p(x, y, z)$. Hence, it is required for the data-based models, either NN for $V(L_{c-3D})$ or TF for $C_p(x, y, z)$, to be updated by additional nodes in NN or higher order in TF due to the additional nonlinearity from coupled PDE. The control algorithms will also be re-designed correspondingly.

However, it is really more realistic if the data-based control algorithms are designed in a 3D scenario. The relevant work will also be achieved in future work.

- As one of the control algorithms, the present design methodology in 2D corner zone is still applicable in 3D domain, if several necessary changes are made. For example, the area of recirculation zone $A(L_{c-2D})$ is modified to volume $V(L_{c-3D})$ in 3D as a control medium, and the local particle concentration $C_p(x, y, z)$ may be defined as the ratio of the residual particle number to a given small controlled volume, namely $N_p(x, y, z)/V_0$.

Other ideas for the potential extension of current work are listed as follows.

- It would be interesting to improve the present two-phase flow models with consideration of more coupled physical and biological effects on the flow, such as thermal effect of wall or particle on the corner flow pattern, biological effect on bioaerosol releasing size and rate, the humidity effect on bioaerosol growth and aerosolization, and phase-change effect on

movement of liquid particles. In addition, the control of aerodynamic-driven bioaerosol releasing rate at boundary layer would be another attractive topic.

- It would be universally practicable if other types of two-phase flow are studied in the future work, such that various control objectives could be achieved, for example, data-driven control of the transport efficiency in a liquid-solid slurry flow, and the bubble shape in an gas-liquid bubble flow.
- Better control performance would be achieved if advanced data-driven methods could be implemented for identification of dynamics for two-phase flow model. For example, deep learning algorithm would be employed for a more accurate system identification, due to the capability for strong nonlinearity. Furthermore, other advanced data-driven controller design algorithms for nonlinear systems could be considered in future studies, such as learning-based or genetic-based controller.
- The open-loop control strategies are implemented in this study. For an accurate controller design and real control problem, it would be academically and practically worthy to develop feedback control laws for improvement of control accuracy and real-time supervision capability of discrete-phase movement. Therefore, online modeling techniques, the location of the sensors, and real-time controller algorithm would be studied in the future. Moreover, it is also noteworthy that the more discussion on PID control should be conducted in the future due to its wide application in industrial processes.
- The present research theoretically focuses on the control of discrete phase concentration for a two-phase flow. Therefore, it is worthwhile to conduct

experiment by the guideline developed by the present numerical simulations, including the state-of-art experimental studies for validation of theoretical two-phase corner flow modeling and for design of controller with proper actuator.

References

- [1] Elger, D. F.; Roberson, J. A., *Engineering Fluid Mechanics*. Wiley Hoboken: New York, 2013.
- [2] Kundu, P. K., *Fluid Mechanics*. 5th ed.; Academic Press: London, 2011.
- [3] Rubin, S. G., Incompressible flow along a corner. *Journal of Fluid Mechanics* **2006**, 26 (01), 97-110.
- [4] Reilly, K.; Wilkinson, D. P.; Taghipour, F., Photocatalytic water splitting in a fluidized bed system: computational modeling and experimental studies. *Applied Energy* **2018**, 222, 423-436.
- [5] Huang, X.; Wang, X.; Liao, G., Visualization of two phase flow inside an effervescent atomizer. *Journal of Visualization* **2008**, 11 (4), 299-308.
- [6] Wittner, M. O.; Karbstein, H. P.; Gaukel, V., Spray performance and steadiness of an effervescent atomizer and an air-core-liquid-ring atomizer for application in spray drying processes of highly concentrated feeds. *Chemical Engineering and Processing - Process Intensification* **2018**, 128, 96-102.
- [7] Yan, Y.; Li, X.; Ito, K., Numerical investigation of indoor particulate contaminant transport using the Eulerian-Eulerian and Eulerian-Lagrangian two-phase flow models. *Experimental and Computational Multiphase Flow* **2019**, 2 (1), 31-40.
- [8] Crowe, C. T.; Schwarzkopf, J. D.; Sommerfeld, M.; Tsuji, Y., *Multiphase Flows with Droplets and Particles*. Chemical Rubber Company Press: Boca Raton, 2011.
- [9] Brennen, C. E., *Fundamentals of Multiphase Flow*. Cambridge University Press: Cambridge, 2005.
- [10] Lee, C. F., *Introduction to Multiphase Flows*. Department of Bioengineering, Imperial College: London, 2015.
- [11] Shui, L.; Eijkel, J. C.; van den Berg, A., Multiphase flow in microfluidic systems --control and applications of droplets and interfaces. *Advances in Colloid and Interface Science* **2007**, 133 (1), 35-49.
- [12] Kolev, N. I., *Multiphase Flow Dynamics 5*. 3rd ed.; Springer International Publishing: Cham, 2015; Vol. 9783642206016.
- [13] Sun, W.; Zhong, W.; Echehki, T., Large eddy simulation of non-premixed pulverized coal combustion in corner-fired furnace for various excess air ratios. *Applied Mathematical Modelling* **2019**, 74, 694-707.

- [14] Wang, S.; Wu, G.; Wang, Y.; Zhou, Y.; Qi, H.; Li, D., CFD for multiphase flow transport of buried crude oil pipeline leakage. *2012 International Conference on Pipelines and Trenchless Technology* **2012**, 861-874.
- [15] Heijnen, J. J.; Mulder, A.; Enger, W.; Hoeks, F., Review on the application of anaerobic fluidized bed reactors in waste-water treatment. *The Chemical Engineering Journal* **1989**, *41* (3), B37-B50.
- [16] Zhang, C.; Ma, Y., *Ensemble Machine Learning: Methods and Applications*. Springer: Verlag New York, 2012; p 1-329.
- [17] Fung, R. F.; Lin, F. J.; Wai, R. J.; Lu, P. Y., Fuzzy neural network control of a motor-quick-return servomechanism. *Mechatronics* **2000**, *10* (1), 145-167.
- [18] Brunton, S. L.; Noack, B. R.; Koumoutsakos, P., Machine learning for fluid mechanics. *Annual Review of Fluid Mechanics* **2020**, *52* (1), 477-508.
- [19] Dietterich, T. G. Machine learning for sequential data: a review. *Structural, Syntactic, and Statistical Pattern Recognition*, Berlin, Heidelberg, 2002//; Caelli, T.; Amin, A.; Duin, R. P. W.; de Ridder, D.; Kamel, M., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 2002; pp 15-30.
- [20] Wang, Y.; Yu, Y.; Cao, S.; Zhang, X.; Gao, S., A review of applications of artificial intelligent algorithms in wind farms. *Artificial Intelligence Review* **2019**, *53*, 3447–3500.
- [21] Wang, Z.; Chen, Y., Data-driven modeling of building thermal dynamics: methodology and state of the art. *Energy and Buildings* **2019**, *203*, 109405.
- [22] Newhart, K. B.; Holloway, R. W.; Hering, A. S.; Cath, T. Y., Data-driven performance analyses of wastewater treatment plants: a review. *Water Research* **2019**, *157*, 498-513.
- [23] Zarra, T.; Galang, M. G.; Ballesteros, F.; Belgiorno, V.; Naddeo, V., Environmental odour management by artificial neural network – a review. *Environment International* **2019**, *133*, 105189.
- [24] Leiner, T.; Rueckert, D.; Suinesiaputra, A.; Baeßler, B.; Nezafat, R.; Išgum, I.; Young, A. A., Machine learning in cardiovascular magnetic resonance: basic concepts and applications. *Journal of Cardiovascular Magnetic Resonance* **2019**, *21* (1), 61.
- [25] Patil, S.; Awan, K.; Arakeri, G.; Seneviratne, C.; Muddur, N.; Malik, S.; Ferrari, M.; Brennan, P., Machine learning and its potential applications to the genomic study of head and neck cancer—a systematic review. *Journal of Oral Pathology & Medicine* **2019**, 48.

- [26] Wang, C.; Zhu, X.; Hong, J.; Zheng, D., Artificial intelligence in radiotherapy treatment planning: present and future. *Technology in Cancer Research & Treatment* **2019**, *18*, 153303381987392.
- [27] Huang, S.; Li, Z.; Liu, Y.; Dashaung, G.; Zhang, X.; Hao, J.; Yang, F., Neural regulation of bone remodeling: identifying novel neural molecules and pathways between brain and bone. *Journal of Cellular Physiology* **2018**, *234*.
- [28] M.V, S.; C.K, B., Online voltage stability assessment of power system by comparing voltage stability indices and extreme learning machine. *International Conference on Swarm, Evolutionary, and Memetic Computing, Springer* **2013**, 710-724.
- [29] Cheng, L.; Tao, Y. U., A new generation of AI: a review and perspective on machine learning technologies applied to smart energy and electric power systems. *International Journal of Energy Research* **2019**, *43*.
- [30] Latah, M.; Toker, L., Artificial intelligence enabled software defined networking: a comprehensive overview. *Institution of Engineering and Technology Networks* **2018**, *8*.
- [31] Jones, A. P., Indoor air quality and health. *Atmospheric Environment* **1999**, *33* (28), 4535-4564.
- [32] National Research, C., *Indoor Pollutants*. The National Academies Press: Washington, DC, 1981.
- [33] Brągoszewska, E.; Mainka, A.; Pastuszka, J., Bacterial and fungal aerosols in rural nursery schools in southern Poland. *Atmosphere* **2016**, *7* (11), 142.
- [34] Kotzias, D., Indoor air and human exposure assessment – needs and approaches. *Experimental and Toxicologic Pathology* **2005**, *57*, 5-7.
- [35] Hussin, N. H. M.; Sann, L. M.; Shamsudin, M. N.; Hashim, Z., Characterization of bacteria and fungi bioaerosol in the indoor air of selected primary schools in Malaysia. *Indoor and Built Environment* **2011**, *20* (6), 607-617.
- [36] Okten, S.; Asan, A., Airborne fungi and bacteria in indoor and outdoor environment of the Pediatric Unit of Edirne Government Hospital. *Environ Monit Assess* **2012**, *184* (3), 1739-51.
- [37] Nazaroff, W. W., Indoor bioaerosol dynamics. *Indoor Air* **2016**, *26* (1), 61-78.
- [38] Nazaroff, W. W., Indoor particle dynamics. *Indoor Air* **2004**, *14* (Supplement 7), 175-83.

- [39] Douwes, J.; Thorne, P.; Pearce, N.; Heederik, D., Bioaerosol health effects and exposure assessment: progress and prospects. *Annals of Occupational Hygiene* **2003**, 47 (3), 187-200.
- [40] Srikanth, P.; Sudharsanam, S.; Steinberg, R., Bio-aerosols in indoor environment: composition, health effects and analysis. *Indian Journal of Medical Microbiology* **2008**, 26 (4), 302-12.
- [41] Pasanen, A. L., A review: fungal exposure assessment in indoor environments. *Indoor Air* **2001**, 11 (2), 87-98.
- [42] Samadi, S.; Wouters, I. M.; Heederik, D. J., A review of bio-aerosol exposures and associated health effects in veterinary practice. *Annals of Agricultural and Environmental Medicine* **2013**, 20 (2), 206-21.
- [43] Pope, C. A.; Dockery, D. W., Health effects of fine particulate air pollution: lines that connect. *Journal of the Air & Waste Management Association* **2006**, 56 (6), 709-42.
- [44] Lee, B. H.; Yee, S. W.; Kang, D. H.; Yeo, M. S.; Kim, K. W., Multi-zone simulation of outdoor particle penetration and transport in a multi-story building. *Building Simulation* **2016**, 10 (4), 525-534.
- [45] Hyeun Jun, M.; Young Ran, Y., Investigation of physical characteristics of houses and occupants' behavioural factors for mould infestation in residential buildings. *Indoor and Built Environment* **2010**, 19 (1), 57-64.
- [46] Fernandez, G.; Mendina, M.; Usera, G., Heterogeneous computing (CPU–GPU) for pollution dispersion in an urban environment. *Computation* **2020**, 8 (1).
- [47] Joseph, D. D., Potential flow of viscous fluids: historical notes. *International Journal of Multiphase Flow* **2006**, 32 (3), 285-310.
- [48] Yin, J.; Qian, Y.; Zhang, T.; Wang, D., Numerical investigation on the bubble separation in a gas-liquid separator applied in TMSR. *Annals of Nuclear Energy* **2018**, 114, 122-128.
- [49] Saffman, P. G., *Vortex Dynamics*. Cambridge University Press: Cambridge, 1992.
- [50] Kuwahara, K., Study of flow past a circular cylinder by an inviscid model. *Journal of the Physical Society of Japan* **1978**, 45 (1), 292-297.
- [51] Kuwahara, K., Numerical study of flow past an inclined flat plate by an inviscid model. *Journal of the Physical Society of Japan* **1973**, 35 (5), 1545-1551.

- [52] Sarpkaya, T.; Schoaff, R. L., Inviscid model of two-dimensional vortex shedding by a circular cylinder. *American Institute of Aeronautics and Astronautics Journal* **1979**, *17* (11), 1193-1200.
- [53] Clements, R. R., An inviscid model of two-dimensional vortex shedding. *Journal of Fluid Mechanics* **1973**, *57* (2), 321-336.
- [54] Epureanu, B. I.; Hall, K. C.; Dowell, E. H., Reduced-order models of unsteady viscous flows in turbomachinery using viscous-inviscid coupling. *Journal of Fluids and Structures* **2001**, *15* (2), 255-273.
- [55] Hafez, M.; Shatalov, A.; Nakajima, M., Improved numerical simulations of incompressible flows based on viscous/inviscid interaction procedures. *Computers & Fluids* **2007**, *36* (10), 1588-1591.
- [56] Korakianitis, T., On the propagation of viscous wakes and potential flow in axial-turbine cascades. *Journal of Turbomachinery* **1993**, *115* (1), 118-127.
- [57] van Esch, B. P. M.; Kruyt, N. P., Hydraulic performance of a mixed-flow pump: unsteady inviscid computations and loss models. *Journal of Fluids Engineering* **2001**, *123* (2), 256-264.
- [58] Avramov, K. V.; Papazov, S. V.; Breslavsky, I. D., Dynamic instability of shallow shells in three-dimensional incompressible inviscid potential flow. *Journal of Sound and Vibration* **2017**, *394*, 593-611.
- [59] Benjamin, T. B., Wave formation in laminar flow down an inclined plane. *Journal of Fluid Mechanics* **1957**, *2* (6), 554-573.
- [60] Abushammala, O.; Hreiz, R.; Lemaître, C.; Favre, É., Laminar flow friction factor in highly curved helical pipes: numerical investigation, predictive correlation and experimental validation using a 3D-printed model. *Chemical Engineering Science* **2019**, *207*, 1030-1039.
- [61] Liu, Y.; Li, J.; Smits, A. J., Roughness effects in laminar channel flow. *Journal of Fluid Mechanics* **2019**, *876*, 1129-1145.
- [62] Yadav, U.; Chandra, L.; Bandyopadhyay, B., Hydraulically and thermally developing laminar flow induced isolated inelastic particle transport and deposition on a flat plate. *Solar Energy* **2019**, *188*, 1298-1305.
- [63] Su, L.; Duan, Z.; He, B.; Ma, H.; Ding, G., Laminar flow and heat transfer in the entrance region of elliptical minichannels. *International Journal of Heat and Mass Transfer* **2019**, *145*, 118717.
- [64] Chai, L.; Xia, G. D.; Wang, H. S., Laminar flow and heat transfer characteristics of interrupted microchannel heat sink with ribs in the transverse microchambers. *International Journal of Thermal Sciences* **2016**, *110*, 1-11.

- [65] Mukherjee, S.; Gupta, A. K.; Chhabra, R. P., Laminar forced convection in power-law and Bingham plastic fluids in ducts of semi-circular and other cross-sections. *International Journal of Heat and Mass Transfer* **2017**, *104*, 112-141.
- [66] Renksizbulut, M.; Niazmand, H., Laminar flow and heat transfer in the entrance region of trapezoidal channels with constant wall temperature. *Journal of Heat Transfer* **2005**, *128* (1), 63-74.
- [67] Shi, H.; Di Miceli Raimondi, N.; Fletcher, D. F.; Cabassud, M.; Gourdon, C., Numerical study of heat transfer in square millimetric zigzag channels in the laminar flow regime. *Chemical Engineering and Processing - Process Intensification* **2019**, *144*, 107624.
- [68] Bashir, A. I.; Everts, M.; Bennacer, R.; Meyer, J. P., Single-phase forced convection heat transfer and pressure drop in circular tubes in the laminar and transitional flow regimes. *Experimental Thermal and Fluid Science* **2019**, *109*, 109891.
- [69] Haussmann, M.; Barreto, A. C.; Kouyi, G. L.; Rivière, N.; Nirschl, H.; Krause, M. J., Large-eddy simulation coupled with wall models for turbulent channel flows at high Reynolds numbers with a lattice Boltzmann method — application to Coriolis mass flowmeter. *Computers & Mathematics with Applications* **2019**, *78* (10), 3285-3302.
- [70] Peters, B.; Pozzetti, G., Numerical analysis of powder deposition in direct material injection. *Granular Matter* **2019**, *22* (1), 2.
- [71] Zhang, J.; Yang, X.; Sun, L.; Liu, S., Evaluation of vortex sheet on agglomerating and blocking fine dust in turbulence area. *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects* **2020**, *42* (2), 233-245.
- [72] Wei, S.; Jafaryar, M.; Sheikholeslami, M.; Shafee, A.; Nguyen-Thoi, T.; Yazdani, T. M.; Tlili, I.; Li, Z., Simulation of nanomaterial turbulent modeling in appearance of compound swirl device concerning exergy drop. *Physica A: Statistical Mechanics and its Applications* **2019**, *534*, 122121.
- [73] Rath, S.; Dash, S. K., Numerical study of laminar and turbulent natural convection from a stack of solid horizontal cylinders. *International Journal of Thermal Sciences* **2020**, *148*, 106147.
- [74] Gu, W.; He, J.; Wang, D.; He, Y., The transport and decay of radioactive aerosols in a wall-bounded turbulent flow. *Annals of Nuclear Energy* **2019**, *134*, 125-133.
- [75] Kim, J. H.; Jeong, S. W.; Ahn, B. K., Numerical and experimental study on unsteady behavior of cavitating flow around a two-dimensional wedge-shaped body. *Journal of Marine Science and Technology* **2019**, *24* (4), 1256-1264.

- [76] Shui, L.; Eijkel, J.; Vandenberg, A., Multiphase flow in micro- and nanochannels. *Sensors and Actuators B: Chemical* **2007**, *121* (1), 263-276.
- [77] Huh, D.; Tung, Y.-C.; Wei, H.-H.; Grotberg, J. B.; Skerlos, S. J.; Kurabayashi, K.; Takayama, S., Use of air-liquid two-phase flow in hydrophobic microfluidic channels for disposable flow cytometers. *Biomedical Microdevices* **2002**, *4* (2), 141-149.
- [78] Noack, B. R.; Mezić, I.; Tadmor, G.; Banaszuk, A., Optimal mixing in recirculation zones. *Physics of Fluids* **2004**, *16* (4), 867-888.
- [79] Noack, B. R.; Mezic, I.; Banaszuk, A., Controlling vortex motion and chaotic advection. *Proceedings of the 39th Institute of Electrical and Electronics Engineers Conference on Decision and Control* **2000**, *2*, 1716-1723.
- [80] Suh, Yong K., Periodic motion of a point vortex in a corner subject to a potential flow. *Journal of the Physical Society of Japan* **1993**, *62* (10), 3441-3445.
- [81] Deliceoğlu, A.; Çelik, E.; Gürçan, F., Singular treatment of viscous flow near the corner by using matched eigenfunctions. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science* **2018**, *233* (5), 1660-1676.
- [82] Chung, K. M.; Su, K.-C., An experimental study on transonic swept convex-corner flows. *Aerospace Science and Technology* **2019**, *84*, 565-569.
- [83] Maxey, M. R.; Riley, J. J., Equation of motion for a small rigid sphere in a nonuniform flow. *The Physics of Fluids* **1983**, *26* (4), 883-889.
- [84] Xiangnan, Y., *The Foundation of Solid-fluid Flow*. Petroleum Industry Press: Beijing, 1996.
- [85] Mei, R., An approximate expression for the shear lift force on a spherical particle at finite reynolds number. *International Journal of Multiphase Flow* **1992**, *18* (1), 145-147.
- [86] Yu, H. C.; Mui, K. W.; Wong, L. T., Numerical simulation of bioaerosol particle exposure assessment in office environment from MVAC systems. *The Journal of Computational Multiphase Flows* **2017**, *10* (2), 59-71.
- [87] Vegendla, S. N. P.; Heynderickx, G. J.; Marin, G. B., Comparison of Eulerian–Lagrangian and Eulerian–Eulerian method for dilute gas–solid flow with side inlet. *Computers & Chemical Engineering* **2011**, *35* (7), 1192-1199.
- [88] Zhuang, C.; Yang, G.; Long, T.; Hu, D., Numerical comparison of removal and deposition for fully-distributed particles in central- and split-type air-conditioning rooms. *Building and Environment* **2017**, *112*, 17-28.

- [89] Wickman, H. H., Deposition, adhesion, and release of bioaerosols. *Atmospheric Microbial Aerosols*, Lighthart, B.; Mohr, A. J., Eds. Springer US: Boston, MA, 1994; pp 99-165.
- [90] Tian, Z. F.; Tu, J. Y.; Yeoh, G. H., Numerical simulation and validation of dilute gas-particle flow over a backward-facing step. *Aerosol Science and Technology* **2005**, *39* (4), 319-332.
- [91] Zhao, B.; Yang, C.; Yang, X.; Liu, S., Particle dispersion and deposition in ventilated rooms: testing and evaluation of different Eulerian and Lagrangian models. *Building and Environment* **2008**, *43* (4), 388-397.
- [92] Ruck, B.; Makiola, B., Particle dispersion in a single-sided backward-facing step flow. *International Journal of Multiphase Flow* **1988**, *14* (6), 787-800.
- [93] Bewley, T. R., Flow control: new challenges for a new Renaissance. *Progress in Aerospace Sciences* **2001**, *37* (1), 21-58.
- [94] Bewley, T. R.; Moin, P.; Temam, R., DNS-based predictive control of turbulence: an optimal benchmark for feedback algorithms. *Journal of Fluid Mechanics* **2001**, *447*, 179-225.
- [95] Bewley, T. R.; Aamo, O. M., A ‘win-win’ mechanism for low-drag transients in controlled two-dimensional channel flow and its implications for sustained drag reduction. *Journal of Fluid Mechanics* **2004**, *499*, 183-196.
- [96] Aamo, O. M.; Krstić, M.; Bewley, T. R., Control of mixing by boundary feedback in 2D channel flow. *Automatica* **2003**, *39* (9), 1597-1606.
- [97] Bewley, T. R.; Temam, R.; Ziane, M., A general framework for robust control in fluid mechanics. *Physica D: Nonlinear Phenomena* **2000**, *138* (3), 360-392.
- [98] Cathalifaud, P.; Bewley, T. R., A noncausal framework for model-based feedback control of spatially developing perturbations in boundary-layer flow systems. Part I: formulation. *Systems & Control Letters* **2004**, *51* (1), 1-13.
- [99] Sen, M.; Shan, H. S., A review of electrochemical macro- to micro-hole drilling processes. *International Journal of Machine Tools and Manufacture* **2005**, *45* (2), 137-152.
- [100] Mamonova, E. E.; Soudakov, V. G.; Voyevodin, A. V., Vortex flow on the wing of aircraft and flow control to improve lift properties. *Journal of Physics: Conference Series* **2019**, *1268*, 012067.
- [101] dos Santos, G. H.; Mendes, N.; Philippi, P. C., A building corner model for hygrothermal performance and mould growth risk analyses. *International Journal of Heat and Mass Transfer* **2009**, *52* (21-22), 4862-4872.

- [102] Joslin, R. D., Aircraft laminar flow control. *Annual Review of Fluid Mechanics* **1998**, 30 (1), 1-29.
- [103] Loscertales, I. G.; Barrero, A.; Guerrero, I.; Cortijo, R.; Marquez, M.; Gañán-Calvo, A. M., Micro/nano encapsulation via electrified coaxial liquid jets. *Science* **2002**, 295 (5560), 1695.
- [104] Utada, A. S.; Lorenceau, E.; Link, D. R.; Kaplan, P. D.; Stone, H. A.; Weitz, D. A., Monodisperse double emulsions generated from a microcapillary device. *Science* **2005**, 308 (5721), 537.
- [105] Link, D. R.; Anna, S. L.; Weitz, D. A.; Stone, H. A., Geometrically mediated breakup of drops in microfluidic devices. *Physical Review Letters* **2004**, 92 (5), 054503.
- [106] Peulon, S.; Guillou, V.; L'Her, M., Liquid | liquid microinterface. Localization of the phase boundary by voltammetry and chronoamperometry; influence of the microchannel dimensions on diffusion. *Journal of Electroanalytical Chemistry* **2001**, 514 (1), 94-102.
- [107] Garstecki, P.; Fuerstman, M. J.; Whitesides, G. M., Nonlinear dynamics of a flow-focusing bubble generator: an inverted dripping faucet. *Physical Review Letters* **2005**, 94 (23), 234502.
- [108] Khan, S. A.; Günther, A.; Schmidt, M. A.; Jensen, K. F., Microfluidic synthesis of colloidal silica. *Langmuir* **2004**, 20 (20), 8604-8611.
- [109] Kim, J.; Bewley, T. R., A linear systems approach to flow control. *Annual Review of Fluid Mechanics* **2006**, 39 (1), 383-417.
- [110] Huang, S.-C.; Kim, J., Control and system identification of a separated flow. *Physics of Fluids* **2008**, 20 (10), 101509.
- [111] Karaca, H.; Özen, G.; Kasnakoğlu, C., A nonlinear dynamical modeling and control method for the vorticity control of the flow past a circular cylinder. *International Journal of Materials, Mechanics and Manufacturing* **2013**, 324-346.
- [112] Debbagh, K.; Cathalifaud, P.; Airiau, C., Optimal and robust control of small disturbances in a channel flow with a normal magnetic field. *Physics of Fluids* **2007**, 19 (1), 014103.
- [113] Zeng, W.; Li, S.; Wang, Z., Closed-loop feedback control of droplet formation in a T-junction microdroplet generator. *Sensors and Actuators A: Physical* **2015**, 233, 542-547.
- [114] Li, Y. J.; Li, Y.; Cao, T.; Qin, K. R., Transport of dynamic biochemical signals in steady flow in a shallow Y-shaped microfluidic channel: effect of transverse diffusion and longitudinal dispersion. *Journal of Biomechanical Engineering* **2013**, 135 (12), 121011–121019.

- [115] Duraisamy, K.; Iaccarino, G.; Xiao, H., Turbulence modeling in the age of data. *Annual Review of Fluid Mechanics* **2019**, 51 (1), 357-377.
- [116] Kutz, J. N., Deep learning in fluid dynamics. *Journal of Fluid Mechanics* **2017**, 814, 1-4.
- [117] Singh, A. P.; Medida, S.; Duraisamy, K., Machine-learning-augmented predictive modeling of turbulent separated flows over airfoils. *American Institute of Aeronautics and Astronautics Journal* **2017**, 55 (7), 2215-2227.
- [118] Duraisamy, K.; Zhang, Z. J.; Singh, A. P., New approaches in turbulence and transition modeling using data-driven techniques. *53rd American Institute of Aeronautics and Astronautics Aerospace Sciences Meeting* **2015**, 1284.
- [119] Tracey, B. D.; Duraisamy, K.; Alonso, J. J., A machine learning strategy to assist turbulence model development. *53rd American Institute of Aeronautics and Astronautics Aerospace Sciences Meeting* **2015**, 1287.
- [120] Amini, S.; Mohaghegh, S., Application of machine learning and artificial intelligence in proxy modeling for fluid flow in porous media. *Fluids* **2019**, 4, 126.
- [121] Uddin, G. M.; Arafat, S. M.; Kazim, A. H.; Farhan, M.; Niazi, S. G.; Hayat, N.; Zeid, I.; Kamarthi, S., Artificial intelligence-based Monte-Carlo numerical simulation of aerodynamics of tire grooves using computational fluid dynamics. *Artificial Intelligence for Engineering Design, Analysis and Manufacturing* **2019**, 33 (3), 302-316.
- [122] Zabihi, R.; Mowla, D.; Karami, H. R., Artificial intelligence approach to predict drag reduction in crude oil pipelines. *Journal of Petroleum Science and Engineering* **2019**, 178, 586-593.
- [123] Guo, X.; Li, W.; Iorio, F., Convolutional neural networks for steady flow approximation. *The 22nd International Conference on Knowledge Discovery and Data Mining* **2016**, 481-490.
- [124] An, Y. J.; Yoo, K. H.; Na, M. G.; Kim, Y. S., Critical flow prediction using simplified cascade fuzzy neural networks. *Annals of Nuclear Energy* **2020**, 136, 107047.
- [125] Wang, Z.; Xiao, D.; Fang, F.; Govindan, R.; Pain, C. C.; Guo, Y., Model identification of reduced order fluid dynamics systems using deep learning. *International Journal for Numerical Methods in Fluids* **2018**, 86 (4), 255-268.
- [126] Wu, J. L.; Xiao, H.; Paterson, E., Physics-informed machine learning approach for augmenting turbulence models: a comprehensive framework. *Physical Review Fluids* **2018**, 3 (7), 074602.

- [127] Wang, J. X.; Wu, J. L.; Xiao, H., Physics-informed machine learning approach for reconstructing Reynolds stress modeling discrepancies based on DNS data. *Physical Review Fluids* **2017**, 2 (3), 034603.
- [128] Ling, J.; Kurzawski, A.; Templeton, J., Reynolds averaged turbulence modelling using deep neural networks with embedded invariance. *Journal of Fluid Mechanics* **2016**, 807, 155-166.
- [129] Fu, K., Learning control systems-review and outlook. *Institute of Electrical and Electronics Engineers Transactions on Pattern Analysis and Machine Intelligence* **1986**, PAMI-8 (3), 327-342.
- [130] Chen, Y.; Meng, T.; Wang, Y.; Wang, K.; Meng, S.; Huang, D., Iterative learning control of two-phase laminar flow interface in Y-shaped microfluidic channel. *Institute of Electrical and Electronics Engineers Transactions on Control Systems Technology* **2019**, 27 (6), 2743-2748.
- [131] Gautier, N.; Aider, J. L.; Duriez, T.; Noack, B. R.; Segond, M.; Abel, M., Closed-loop separation control using machine learning. *Journal of Fluid Mechanics* **2015**, 770, 442-457.
- [132] Lee, C.; Kim, J.; Babcock, D.; Goodman, R., Application of neural networks to turbulence control for drag reduction. *Physics of Fluids* **1997**, 9 (6), 1740-1747.
- [133] Yue, J.; Xu, K. J.; Liu, W.; Zhang, J. G.; Fang, Z. Y.; Zhang, L.; Xu, H. R., SVM based measurement method and implementation of gas-liquid two-phase flow for CMF. *Measurement* **2019**, 145, 160-171.
- [134] Buist, J.; Sanderse, B.; Halder van, Y.; Koren, B.; Heijst, G. Machine learning for closure models in multiphase flow applications. *3rd European Community on Computational Methods in Applied Sciences Thematic Conference on Uncertainty Quantification in Computational Sciences and Engineering*, 2019; pp 379-399.
- [135] Wang, W.; Sefiane, K.; Duursma, G.; Liang, X.; Chen, Y., Void fraction measurement of gas-liquid two-phase flow based on empirical mode decomposition and artificial neural networks. *Heat Transfer Engineering* **2019**, 40 (16), 1403-1416.
- [136] Zhou, Y.; Chen, F.; Sun, B., Identification method of gas-liquid two-phase flow regime based on image multi-feature fusion and support vector machine. *Chinese Journal of Chemical Engineering* **2008**, 16 (6), 832-840.
- [137] Grüne, L.; Pannek, J., Nonlinear model predictive control. *Nonlinear model predictive control: theory and algorithms*, Grüne, L.; Pannek, J., Eds. Springer London: London, 2011; pp 43-66.

- [138] Ławryńczuk, M., Neural networks in model predictive control. *Intelligent Systems for Knowledge Management*, Nguyen, N. T.; Szczerbicki, E., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 2009; pp 31-63.
- [139] Ławryńczuk, M., Predictive control of a distillation column using a control-oriented neural model. *Adaptive and Natural Computing Algorithms*, Dobnikar, A.; Lotrič, U.; Šter, B., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 2011; pp 230-239.
- [140] Ławryńczuk, M. Nonlinear predictive control based on multivariable neural wiener models. *Adaptive and Natural Computing Algorithms*, Berlin, Heidelberg, 2011//; Dobnikar, A.; Lotrič, U.; Šter, B., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 2011; pp 31-40.
- [141] Janakiraman, V. M.; Nguyen, X.; Assanis, D., An ELM based predictive control method for HCCI engines. *Engineering Applications of Artificial Intelligence* **2016**, 48, 106-118.
- [142] Janakiraman, V. M.; Nguyen, X.; Assanis, D., Nonlinear model predictive control of a gasoline HCCI engine using extreme learning machines. *Special Issue on Neurodynamic Systems for Optimization and Applications* **2015**.
- [143] Santos, P.; Pitarch, J. L.; Vicente, A.; de Prada, C.; García, Á., Improving operation in an industrial MDF flash dryer through physics-based NMPC. *Control Engineering Practice* **2020**, 94, 104213.
- [144] Peng, Z.; Hu, J.; Shi, K.; Luo, R.; Huang, R.; Ghosh, B. K.; Huang, J., A novel optimal bipartite consensus control scheme for unknown multi-agent systems via model-free reinforcement learning. *Applied Mathematics and Computation* **2020**, 369, 124821.
- [145] Garg, D.; Chli, M.; Vogiatzis, G., Deep reinforcement learning for autonomous traffic light control. *2018 3rd IEEE International Conference on Intelligent Transportation Engineering (ICITE)* **2018**, 214-218.
- [146] Elsrogy, W. M.; Fkirin, M. A.; Hassan, M. A. M., Speed control of DC motor using PID controller based on artificial intelligence techniques. *2013 International Conference on Control, Decision and Information Technologies* **2013**, 196-201.
- [147] Prabhu, S. M.; Garg, D. P., Artificial neural network based robot control: an overview. *Journal of Intelligent and Robotic Systems* **1996**, 15 (4), 333-365.
- [148] Albus, J. S., Data storage in the cerebellar model articulation controller (CMAC). *Journal of Dynamic Systems, Measurement, and Control* **1975**, 97 (3), 228-233.

- [149] Widrow, B., Adaptive inverse control. *International Federation of Automatic Control Proceedings Volumes* **1987**, 20 (2), 1-5.
- [150] Jordan, M. I. *Supervised Learning and Systems with Excess Degrees of Freedom*; University of Massachusetts: Boston, 1988.
- [151] Saerens, M.; Soquet, A. A neural controller. *1989 First Institute of Electrical and Electronics Engineers International Conference on Artificial Neural Networks*, 16-18 Oct. 1989; 1989; pp 211-215.
- [152] Miller, W., Sensor-based control of robotic manipulators using a general learning algorithm. *Institute of Electrical and Electronics Engineers Journal on Robotics and Automation* **1987**, 3 (2), 157-165.
- [153] Miller, W. T., Real-time application of neural networks for sensor-based control of robots with vision. *Institute of Electrical and Electronics Engineers Transactions on Systems, Man, and Cybernetics* **1989**, 19 (4), 825-831.
- [154] Mensah-Attipoe, J.; Saari, S.; Veijalainen, A. M.; Pasanen, P.; Keskinen, J.; Leskinen, J. T. T.; Reponen, T., Release and characteristics of fungal fragments in various conditions. *Science of the Total Environment* **2016**, 547, 234-243.
- [155] Li, Y.; Jin, X.; Yang, L.; Du, X.; Yang, Y., Indoor and outdoor particle concentration distributions of a typical meeting room during haze and clear-sky days. *Science China Technological Sciences* **2017**, 60 (3), 355-362.
- [156] Madsen, A. M., Effects of airflow and changing humidity on the aerosolization of respirable fungal fragments and conidia of *Botrytis cinerea*. *Applied and Environmental Microbiology* **2012**, 78 (11), 3999-4007.
- [157] Kildeso, J.; Wurtz, H.; Nielsen, K. F.; Kruse, P.; Wilkins, K.; Thrane, U.; Gravesen, S.; Nielsen, P. A.; Schneider, T., Determination of fungal spore release from wet building materials. *Indoor Air* **2003**, 13 (2), 148-155.
- [158] Sun, D.; She, J.; Gower, J.; Stokes, C.; Windham, G.; Baird, R.; Mlsna, T., Effects of growth parameters on the analysis of *aspergillus flavus* volatile metabolites. *Separations* **2016**, 3 (2).
- [159] Nielsen, K. F.; Holm, G.; Uttrup, L. P.; Nielsen, P. A., Mould growth on building materials under low water activities. Influence of humidity and temperature on fungal growth and secondary metabolism. *International Biodeterioration & Biodegradation* **2004**, 54 (4), 325-336.
- [160] Pasanen, A. L.; Pasanen, P.; Jantunen, M. J.; Kalliokoski, P., Significance of air humidity and air velocity for fungal spore release into the air. *Atmospheric Environment. Part A. General Topics* **1991**, 25 (2), 459-462.

- [161] Feigley, C.; Khan, J.; Salzberg, D.; Hussey, J.; Attaway, H.; Steed, L.; Schmidt, M.; Michels, H., Experimental tests of copper components in ventilation systems for microbial control. *Heating, Ventilation, Air-conditioning, and Refrigeration Research* **2013**, *19* (1), 53-62.
- [162] Liu, X.; Zhai, Z., Identification of appropriate CFD models for simulating aerosol particle and droplet indoor transport. *Indoor and Built Environment* **2016**, *16* (4), 322-330.
- [163] Katifori, E.; Alben, S.; Cerda, E.; Nelson, D. R.; Dumais, J., Foldable structures and the natural design of pollen grains. *Proceedings of the National Academy of Sciences of the United States of America* **2010**, *107* (17), 7635-9.
- [164] Van Houdt, R.; Kokkonen, E.; Lehtimäki, M.; Pasanen, P.; Leys, N.; Kulmala, I., Requirements for modeling airborne microbial contamination in space stations. *Acta Astronautica* **2018**, *144*, 380-387.
- [165] Van Impe, J. F.; Poschet, F.; Geeraerd, A. H.; Vereecken, K. M., Towards a novel class of predictive microbial growth models. *International Journal of Food Microbiology* **2005**, *100* (1-3), 97-105.
- [166] Lewis, F. L.; Vrabie, D. L.; Syrmos, V. L., *Optimal Control*. John Wiley & Sons: Hoboken 2012.
- [167] Kundu, P. K.; Cohen, I. M.; Dowling, D. R., *Fluid Mechanics*. Academic Press: London, 2011.
- [168] Lighthart, B.; Mohr, A. J., *Atmospheric Microbial Aerosols: Theory and Applications*. Springer United States: New York, 2012.
- [169] Krupp, H., Particle adhesion theory and experiment. *Advances in Colloid and Interface Science* **1967**, *1* (2), 111-239.
- [170] Julien, P., Concentration of very fine silts in a steady vortex. *Journal of Hydraulic Research* **1986**, *24* (4), 255-264.
- [171] Dorf, R. C., *The Engineering Handbook*. 2nd ed.; Chemical Rubber Company Press: Boca Raton, 2005.
- [172] Cardarelli, F., Cements, concrete, building stones and construction materials. *Materials Handbook*, Cardarelli, F., Ed. Springer London: London, 2008; pp 967-981.
- [173] Ławryńczuk, M., A family of model predictive control algorithms with artificial neural networks. *International Journal of Applied Mathematics and Computer Science* **2007**, *17* (2), 217-232.

- [174] Julien, P. Y., Motion of sediment particles in a Rankine combined vortex. *Civil Engineering Reports, Colorado State University Libraries*; 84/85-6 **1985**.
- [175] Mukherjee, Y. X.; Mukherjee, S., On boundary conditions in the element-free Galerkin method. *Computational Mechanics* **1997**, 19 (4), 264-270.
- [176] Roache, P. J., *Verification and validation in computational science and engineering*. Hermosa Albuquerque, 1998.
- [177] Hellsten, A.; Laine, S.; Hellsten, A.; Laine, S. Extension of the k-omega-SST turbulence model for flows over rough surfaces. *22nd Atmospheric Flight Mechanics Conference*, American Institute of Aeronautics and Astronautics: 1997; p 3577.
- [178] Hellsten, A., Some improvements in Menter's k-omega SST turbulence model. *29th American Institute of Aeronautics and Astronautics, Fluid Dynamics Conference*, American Institute of Aeronautics and Astronautics: 1998; p 2554.
- [179] Menter, F. R.; Kuntz, M.; Langtry, R., Ten years of industrial experience with the SST turbulence model. *Turbulence, Heat and Mass Transfer* **2003**, 4 (1), 625-632.
- [180] Karimi, M.; Akdogan, G.; Dellimore, K. H.; Bradshaw, S. M. Comparison of different drag coefficient correlations in the CFD modelling of a laboratory-scale Rushton-turbine flotation tank. *Ninth International Conference on CFD in the Minerals and Process Industries CSIRO, Melbourne, Australia*, 2012; pp 10-12.

Publications arising from the thesis

Journal Papers

1. **X. Zhang**, H. Li. Feasibility analysis for control of bioaerosol concentration at indoor corner via airflow from ventilation outlet with energy optimization, *Journal of Cleaner Production* 248 (2020) 119289.
2. **X. Zhang**, H. Li, Neutral-network-based control of discrete-phase concentration in a gas-particle corner flow with optimal energy consumption, *Computer & Mathematics with Applications* (2020)10213.
3. T. Fan, S. Park, Q. Shi, **X. Zhang**, Q. Liu, Y. Song, H. Chin, M. S. B. Ibrahim, N. Mokrzecka, Y. Yang, H. Li, J. Song, S. Suresh, N. Cho, Transformation of Hard Pollen into Soft Matter, *Nature Communication* 1449 (2020).
4. **X. Zhang**, H. Li, Development of machine learning based PID controller on a gas-particle turbulent corner flow to remove indoor bioaerosol pollutant (in preparation).
5. **X. Zhang**, S.E. Wredh, H. Li, Machine learning based control of vortex involved two-phase flow by learning the difference between laminar scheme and potential flow assumption (in preparation).

Conference Papers

1. **X. Zhang**, H. Li. Control of small particle movement at a 90 degree corner. 10th International Conference on Computational Methods, (ICCM 2019), July 2019, Singapore. (Keynote speaker)
2. **X. Zhang**, H. Li. Transient Modelling of the Deformation Behavior of a Spherical Hydrogel Immersed in Solutions with Different Concentrations 10th International Conference on Materials for Advanced Technologies (ICMAT2019), June 2019, Singapore. (Oral Presentation)