Surface interactions of aerosols and their impact on infectious disease transmission

You, Siming

2014

You, S. (2014). Surface interactions of aerosols and their impact on infectious disease transmission. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/61765>

<https://doi.org/10.32657/10356/61765>

NANYANG
TECHNOLOGICAL
UNIVERSITY

**SURFACE INTERACTIONS OF
AEROSOLS AND THEIR IMPACT ON
INFECTIOUS DISEASE TRANSMISSION**

YOU SIMING

**SCHOOL OF MECHANICAL AND AEROSPACE
ENGINEERING**

2014

SURFACE INTERACTIONS OF AEROSOLS AND THEIR IMPACT ON INFECTIOUS DISEASE TRANSMISSION

YOU SIMING

School of Mechanical and Aerospace Engineering

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

2014

Acknowledgements

I would like to express my sincere gratitude to my supervisor, Prof. Wan Man Pun for his invaluable advices and great support throughout my study and research work. During every our meeting, he always patiently provides vivid and detailed explanation to clear up my confusion. It is the every critical suggestion from him that guides me heading towards my research target continuously.

I am also thankful to the technician, Mr. Yap Pow Khim in Fluid Mechanics Lab, and other research students or staff (Zingre Kishor Tarachand, Yang Xingguo, Tang Cheng and Poh Zihan) for their assistance during my experiments.

Last but not least, I dedicate this thesis to my beloved parents, You Xilin and Xiong Runlian, and my beloved wife, Wang Hongyan for their unconditional support and love throughout the process of the research which supports me through my difficult times.

Table of contents

Abstract	vi
List of Figures	ix
List of Tables	xv
List of Symbols	xvii
Chapter 1 Introduction	1
1.1 Background	1
1.2 Objectives and scope.....	6
Chapter 2 Literature Review	9
2.1 Overview of indoor infection transmission modes and existing risk assessment schemes	9
2.1.1 Infection transmission modes	9
2.1.2 Existing risk assessment schemes.....	11
2.2 Adhesion force model	12
2.2.1 Mean adhesion force model	13
2.2.2 Adhesion force distribution model.....	16
2.3 Hydrodynamic force	16
2.3.1 Airflow velocity profile	17
2.3.2 Models of hydrodynamic forces	19
2.4 Model of AIPR.....	19
2.4.1 Theoretical model	20
2.4.2 Empirical model.....	24
2.5 WIPR.....	25

2.6 Indoor particle dynamics.....	27
2.6.1 Two-compartment mass balance models	27
2.7 Biological aspect of pathogen.....	34
2.7.1 Persistence of pathogen.....	34
2.7.2 Infective dose	35
2.8 Risk assessment model	36
2.8.1 Wells-Riley model	36
2.8.2 Dose response model	37
2.9 Conclusions.....	38
Chapter 3 Particle Concentration Dynamics in the Ventilation Duct with AIPR40	
3.1 Introduction.....	40
3.2 Model derivation.....	41
3.3 Validation experiments	44
3.3.1 Surface roughness measurement.....	44
3.3.2 Sample preparation by deposition procedure.....	45
3.3.3 Particle resuspension experiments	48
3.4 Results and discussion	52
3.4.1 Model validation	52
3.4.2 Spatial concentration variation after resuspension	55
3.5 Conclusions.....	56
Chapter 4 Experimental Investigation and Modeling of WIPR.....	58
4.1 Introduction.....	58
4.2 Methodology	58
4.2.1 Experimental setup.....	59
4.2.2 Experimental procedure	61

4.2.3 Parameters.....	63
4.3 Data analysis	64
4.3.1 Resuspension rate calculation	64
4.3.2 Airborne particle concentration model involved with walking	68
4.4 Results and discussion	69
4.4.1 Investigations of factors and mechanisms affecting WIPR	69
4.4.2 Airborne particle concentration modelling	76
4.5 Conclusions.....	79
Chapter 5 Indoor Particle Concentration Models Considering Particle Resuspension Processes	
5.1 Introduction.....	81
5.2 Model development	81
5.2.1 Emission dynamics	82
5.2.2 Model derivation.....	85
5.3 Model validation	89
5.4 Conclusions.....	96
Chapter 6 Risk Assessment Scheme for Infection Transmission Indoors Considering Resuspension Processes	
6.1 Introduction.....	97
6.2 Exposure analysis model.....	97
6.3 Dose response model	100
6.4 Case Study	100
6.4.1 Case 1.....	101
6.4.2 Case 2.....	108
6.5 Conclusions.....	110

Chapter 7 Development of Mean Adhesion Force Model	112
7.1 Introduction.....	112
7.2 Model development	113
7.2.1 Surface roughness	114
7.2.2 Van der Waals force model.....	115
7.2.3 Capillary force model	119
7.3 Model validation	127
7.4 Parameter investigation.....	133
7.4.1 Surface roughness	134
7.4.2 RH.....	137
7.4.3 Contact angle	140
7.4.4 Hurst exponent.....	142
7.5 Conclusions.....	143
Chapter 8 Development of Adhesion Force Distribution Model.....	146
8.1 Introduction.....	146
8.2 Adhesion force distribution model.....	147
8.2.1 Statistical analysis	148
8.2.2 Monte Carlo simulation	150
8.3 Validation experiments	151
8.3.1 RMS roughness measurements	152
8.3.2 Sample preparation	159
8.3.3 Centrifuge experiment	160
8.4 Results and discussion	163
8.4.1 Model validation	163
8.4.2 Effect of RMS roughness distribution on adhesion force distribution ...	170

8.5 Conclusions.....	172
Chapter 9 A New Theoretical Model for AIPR	174
9.1 Introduction.....	174
9.2 Model development	176
9.2.1 Detachment mode of resuspension	176
9.2.2 Hydrodynamic and adhesion forces.....	177
9.2.3 Principle of resuspension model	180
9.3 Results.....	183
9.3.1 Model validation	183
9.4 Conclusions.....	192
Chapter 10 Conclusions and Suggestions for Future Work.....	194
10.1 Conclusions.....	194
10.2 Suggestions for future study	198
Appendix A. Derivation of Eq. (3.4).....	201
Appendix B. Derivation of Eq. (7.13).....	203
Appendix C. Derivation of the Average Radius of Asperity Curvature, Eq. (7.14)	205
Appendix D. Derivation of the Percentage of Area Covered by Meniscus, Eq. (7.33)	207
Appendix E. Comparison of Magnitude of Different Terms in Eq. (7.33) ...	210
Appendix F. Comparison of Predictions between Statistical analysis-based Model and Monte Carlo simulation-based Model.....	212
References.....	213
Publications.....	239

Abstract

Infection transmission has been a major health concern indoors. Exposure analysis and risk analysis are the fundamentals of effectively controlling and managing infection transmission, which requires a clear understanding of transmission mode. A significant fraction of airborne pathogens deposits onto surfaces. Some of these deposited pathogens could be resuspended by airflow or mechanical disturbances and become airborne again, leading to prolonged exposure risk via the airborne mode. Hence, pathogen resuspension can contribute significantly in indoor infection transmission. Understanding the impact of resuspension on infection transmission is crucial for a complete risk assessment scheme. This work intends to improve the current capability of modelling resuspension processes and explore the impact of the resuspension processes on infection transmission by developing a new risk assessment scheme.

Two common types of particle resuspension process relevant to indoor environments were studied, i.e., airflow-induced particle resuspension (AIPR) and walking-induced particle resuspension (WIPR). In the case of AIPR, the particle resuspension in the ventilation duct such as that during a bioterrorist attack was considered. A corresponding model of particle concentration dynamics in the ventilation duct was developed based on the existing empirical resuspension models and was validated against the data of wind tunnel experiments. In the case of WIPR, a scaled resuspension chamber with a pair of model feet installed inside was fabricated to investigate the influence of various factors (e.g., flooring material, particle size,

walking rate, relative humidity and mechanism) towards WIPR. The resuspension rates for WIPR were calculated based on the mass balance model, and the power law was applied to fit the resuspension rate data.

The developed model of particle concentration dynamics in the ventilation duct with AIPR and the power law resuspension rate for WIPR were subsequently substituted into the mass balance models of indoor particle dynamics to develop a set of airborne and surface particle concentration models. Based on the concentration models, a set of inhalational exposure analysis models was developed. Then, a risk assessment scheme was proposed by plugging the exposure analysis into the dose response model. The influence of pathogen resuspension towards infection transmission was examined through two case studies using the developed risk assessment scheme, which generated meaningful insights towards the control and management of infection transmission indoors.

Further effort was put to advance the theoretical AIPR model which has the potential to be used in exposure modelling in the future. A set of mean adhesion force (van der Waals force and capillary force) models was firstly developed. Then, an adhesion force distribution model was developed by integrating the RMS roughness distribution into the mean adhesion force models. Finally, a theoretical AIPR model considering the essential characteristics underlying the process (e.g., turbulent burst, adhesion force distribution, depletion of resuspendable particles and relative humidity) was developed based on the proposed adhesion force distribution model. The new theoretical model is able to predict the effect of humidity on AIPR, which greatly enhances the current capability of modelling AIPR.

List of Figures

Figure 1.1 The knowledge hierarchy of this work.....	6
Figure 2.1 Particle oscillations in different energy balance-based AIPR models.	24
Figure 2.2 A schematic diagram of indoor particle dynamics for mechanical ventilation.	28
Figure 2.3 A schematic diagram of indoor particle dynamics for natural ventilation.	30
Figure 3.1 A schematic diagram of the particle resuspension in a duct.....	43
Figure 3.2 The cumulative size distribution of test particles.	46
Figure 3.3 A schematic diagram of the wind tunnel setup.....	49
Figure 3.4 (a) The boundary layer velocity profiles at various free stream velocities. (b) The relationship between the friction velocity and free stream velocity.....	51
Figure 3.5 The comparison between the measured and modeled concentration variations after particle resuspension for the substrates of (a) aluminum (i: 2 μm ; ii: 4.75 μm), (b) stainless steel (i: 2 μm ; ii: 4.75 μm) and (c) plastic (i: 2 μm ; ii: 4.75 μm). The error bars denote one standard deviation. ...	55
Figure 3.6 The spatial variation of particle concentration in the duct at various time points (10, 20 and 30 s) after resuspension.....	56
Figure 4.1 A schematic diagram of the experimental setup and procedure.	59
Figure 4.2 The sixth order polynomial fitting of the particle concentration variation during Stage 2 for wood PVC under the walking rate of 132	

steps/min (contact case).	65
Figure 4.3 The comparison of the normalized resuspension rates of PM ₁₀ and PM _{2.5} between different materials at the walking rate of 132 steps/min (contact case).	70
Figure 4.4 The comparisons of the normalized resuspension rates of PM ₁₀ between different walking rates for (a) carpet and (b) vinyl (contact case).	72
Figure 4.5 The comparisons of the normalized resuspension rates of PM ₁₀ between different RHs for (a) carpet and (b) vinyl (contact case) at the walking rate of 132 steps/min.	74
Figure 4.6 The comparison of the normalized resuspension rates of PM ₁₀ between the contact case and aerodynamic case for carpet and wood PVC at the walking rate of 132 steps/min.	76
Figure 4.7 The comparison between the measured PM10 concentration profiles and modeled ones for different flooring materials at the highest walking rate (contact case).	77
Figure 4.8 The comparison of PM ₁₀ airborne concentration during the walking between the experimental data of Qian et al. [119] and model predictions.	79
Figure 5.1 The comparison between the model predictions and experimental data from the studies of (a) Qian and Ferro [18] (2.5 μm particles), (b) Qian and Ferro [18] (4.5 μm particles), and (c) Ferro et al. [15]. Note that for the parameters not given in the original studies, reference values were firstly found from the previous literatures or Chapter 4. The reference values were generally varied by ±20% to account for their potential uncertainty during	

modeling.	95
Figure 6.1 The modeling results for Sub-case 1: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability.	105
Figure 6.2 The modeling results for Sub-case 2: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability. The results of Sub-case 1 are added for comparison purposes.	107
Figure 6.3 The modeling results for Case 2: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability.	109
Figure 7.1 A schematic diagram of the proposed van der Waals force model.	117
Figure 7.2 A schematic diagram of the proposed capillary force model.	122
Figure 7.3 The comparison between the predictions of the proposed models and the experimental data. The red dash lines specify 1 order of magnitude difference between the model predictions and experimental data, while the black line indicates the perfect match between the model predictions and the experimental data.	133
Figure 7.4 The influence of roughness towards the van der Waals force and capillary force based on the models of this work and the existing studies for (a) RMS roughness range from 0 – 5 nm and (b) RMS roughness range from 0 – 0.15 nm. The constant parameters for modeling are listed in Table 7.1.....	136
Figure 7.5 The influence of RH towards the van der Waals force and capillary force based on the models of this work and the existing studies. The constant parameters for modeling are listed in Table 7.1.	138

Figure 7.6 The influence of contact angle towards the van der Waals force and capillary force based on the models of this work and the existing studies. The constant parameters for modeling are listed in Table 7.1.	141
Figure 7.7 The influence of Hurst exponent towards the van der Waals force and capillary force based on the models of this work. The constant parameters for modeling are listed in Table 7.1.	143
Figure 8.1 A schematic diagram of adhesion force distribution model. ..	148
Figure 8.2 The workflow chart of the adhesion force distribution model by the Monte Carlo simulation.	151
Figure 8.3 The surface roughness characteristic for the substrates of (a) stainless steel, (b) aluminum, and (c) plastic, respectively.....	154
Figure 8.4 The surface RMS roughness data and the corresponding fits of the mean, lower and upper gamma distributions for the substrates of (a) stainless steel, (b) aluminum and (c) plastic, respectively.	156
Figure 8.5 The microscopic image of particles on a stainless steel substrate.	158
Figure 8.6 A schematic diagram of centrifuge method.	161
Figure 8.7 A schematic diagram of (a) an adapter, (b) the centrifuge with four adapters and (c) the centrifuge with the drum rotor capped.	162
Figure 8.8 The microscopic image of particles on the plastic substrate after the centrifuge experiments under different rotational speeds: (a) 0 RPM (before the centrifuge experiment); (b) 1000 RPM; (c) 3000 RPM; (d) 5000 RPM; (e) 7000 RPM.....	163
Figure 8.9 The comparison between the measured adhesion force distributions and the modelled ones for particles on the substrates of (a) stainless steel, (b) aluminum and (c) plastic. The error bar indicates one standard deviation.	

The vertical error bar indicates one standard deviation of measured fraction, while the horizontal error bar indicates the variation of measured adhesion forces caused by the variation of particle size ($146.1 \pm 1.99 \mu\text{m}$), rotational radius ($d \pm 0.01d$) and rotational speed ($\omega_i \pm 0.01\omega_i$)..... 165

Figure 8.10 The comparison of adhesion force distributions between the model predictions and the experimental data of Prokopovich and Perni [74]: (a) glass substrate and (b) silicone substrate. 169

Figure 8.11 The variation of adhesion force distributions resultant from the variation of (a) the mean and (b) standard deviation of RMS roughness distribution. 171

Figure 9.1 A schematic diagram of the rolling detachment mode. 177

Figure 9.2 The cumulative distribution of adhesion force between particles and a surface. 179

Figure 9.3 A schematic diagram of turbulent bursts in the model. 181

Figure 9.4 A schematic diagram of overlapping bursts. (a) The new turbulent burst overlaps with only one previous burst. (b) The new turbulent burst overlaps with 2 or more than 2 previous bursts. Circles 1 and 1' indicate the areas occupied by the previous bursts. Circles 2 indicate the areas occupied by the new burst. Newly occupied area is highlighted by the red shadow lines. 182

Figure 9.5 The measured RMS roughness data and the corresponding fit of the gamma distribution. 185

Figure 9.6 The lognormal adhesion force distributions for (a) $70 \mu\text{m}$ stainless steel particles, $32 \mu\text{m}$ and $72 \mu\text{m}$ glass particles on the glass substrate under the RH of 25% [274]; (b) $70 \mu\text{m}$ stainless steel particles on the glass

substrate under the RH of 36%, 61% and 67%, respectively [260].	188
Figure 9.7 The comparison between the experimental data and the model predictions for (a) 70 μm stainless steel particles, 32 and 72 μm glass particles on the glass substrate under the RH of 25% [274]; (b) 70 μm stainless steel particles on the glass substrate under the RH of 36%, 61% and 67%, respectively [260].	189
Figure 9.8 The lognormal adhesion force distributions for various cases in the study of [212].	191
Figure 9.9 The comparison between the experimental data of [212] and the model predictions.	192
Figure C.1 A schematic of parameters of asperities.	206
Figure E.1 The comparison of the magnitude of different terms in Eq. (7.33) in terms of the variation of (a) surface RMS roughness σ_1 ($\sigma_2=0$ nm, RH=40%, $R_p = 2.5$ μm) and (b) RH ($\sigma_1=0.4$ nm, $\sigma_2=0$ nm).	211
Figure F.1 The comparison of the predictions between the statistical analysis-based model and the Monte Carlo simulation-based model.	212

List of Tables

Table 2.1 Non-dimensional streamwise and spanwise spacings and period of turbulent bursts.....	17
Table 3.1 Parameters required for the normalized resuspension rate estimation.	45
Table 3.2 The deposited mass of particles and the upstream particle concentration	47
Table 3.3 The normalized resuspension rate and deposition velocities of various cases.	53
Table 4.1 Information about power law fittings and initial surface particle concentrations.	68
Table 5.1 Emission dynamics of various sources.	84
Table 5.2 Parameters used for model predictions during the validation.	93
Table 6.1 Parameters for calculating the normalized resuspension rate of AIPR.	102
Table 6.2 Parameters required by modeling for the case study.....	103
Table 7.1 Parameters for the model predictions against the existing experimental data.....	131
Table 8.1 Mechanical and physical properties of various materials	152
Table 8.2 Parameters of the gamma distributions.	157
Table 8.3 Parameters of the gamma roughness distributions for the study of Prokopovich and Perni [74].	167
Table 8.4 Properties of various materials from the study of Prokopovich and	

Perni [74].	167
Table 9.1 Mechanical and physical properties of the materials of particle and substrate in the studies of [212, 260, 274].	185
Table 9.2 Parameters of the gamma distributions for various particles in the studies of [212, 260, 274]	185
Table 9.3 The parameters of adhesion force distributions for various cases in [212, 260, 274].	186

List of Symbols

Nomenclature

a	Contact radius [m]
a'	Effective contact radius [m]
a_1	Entrance rate of outdoor particles [1/s]
a_2	Entrance rate of resuspended particles [1/s]
a_r	Coefficient in power law function of resuspension rate
b_r	Exponent in power law function of resuspension rate
A	Area acted by capillary pressure [m ²]
A_0	Maximum lateral area coverable [m ²]
A_h	Hamaker constant [J]
A_v	Cross sectional area of ventilation duct [m ²]
A_1	Nominal contact area [m ²]
A_2	Actual contact area [m ²]
b	Loss rate of indoor particles [1/s]
c	Factor related to contact angles
C	Factor accounting for the percentage of nominal contact area
C_0	Particle concentration upstream the resuspension area in the ventilation duct [#/m ³]
C_{t0}	Initial particle concentration in the ventilation duct [#/m ³]
C_c	Particle concentration in the resuspension chamber [μg/m ³] or [#/m ³]
C_i	Indoor airborne particle concentration [μg/m ³] or [#/m ³]
C_o	Outdoor airborne particle concentration [μg/m ³] or [#/m ³]

C_{oc}	Particle concentration outside the resuspension chamber [$\mu\text{g}/\text{m}^3$] or [$\#/\text{m}^3$]
C_{ov}	Airborne particle concentration in the ventilation duct due to AIPR [$\mu\text{g}/\text{m}^3$] or [$\#/\text{m}^3$]
d	Rotational radius [m]
d_{ae}	Aerodynamic diameter of particle [m]
d_p	Particle diameter [m]
d_p^+	Non-dimensional diameter
d_{v1}	Parameter accounting for the effect of particle deposition in the ventilation duct for outdoor particles
d_{v2}	Parameter accounting for the effect of particle deposition in the ventilation duct for the particles from AIPR
d_{v3}	Parameter accounting for the effect of particle deposition in the ventilation duct for the particles in the recirculated air
D	Equilibrium separation distance between solids [m]
D_f	Fractal dimension
E	Indoor constant emission sources besides WIPR
E^*	Composite Young's modulus [Gpa]
E_1	Young's modulus of particle [Gpa]
E_2	Young's modulus of surface [Gpa]
f	Probability density function
f_d	Correction to the Stokes drag
f_p	Fraction of deposited particles belonging to the size bin of d_p
f_{Σ_1}	Probability density function of Σ_1
f_{Σ_2}	Probability density function of Σ_2

f_{X_1}	Probability density function of X_1
f_{X_2}	Probability density function of X_2
f_Y	Probability density function of Y
f'	Adhesion force [N]
f_r'	Fraction of detached particles
F_V	Van der Waals force [N]
F_c	Capillary force [N]
F_{cA}	Critical adhesion force [N]
F_{cA1}	Critical adhesion force corresponding to the mean hydrodynamic detachment forces [N]
F_{cA2}	Critical adhesion force corresponding to the instantaneous hydrodynamic detachment forces [N]
F_A	Total adhesion force [N]
F_d	Detachment force [N]
F_D	Hydrodynamic drag force [N]
F_D^+	Non-dimensional drag force
F_G	Gravitational force [N]
F_L	Hydrodynamic lift force [N]
F_L^+	Non-dimensional lift force
F'	Random variable representing adhesion force
g	Gravitational acceleration [m/s ²]
g_h	Overall height distribution function
g_h'	Height distribution function of the apparent nominally smooth shape
G	Factor accounting for the actually covered area

G'	Characteristic length scale [m]
h	Height of surface asperity [m]
$h_{\min}$	Maximum height of peak [m]
$h_{\max}$	Maximum height of valley [m]
h_l	Height of meniscus [m]
H	Hurst exponent
H_c	Separation distance between the average surface plane and particle caused by surface roughness [m]
$H_{\max}$	Maximum separation distance available for meniscus formation [m]
I	Amount of pathogens human is exposed to
$J_{F'}$	Cumulative probability distribution of F'
l	Length scale of a fractal asperity [m]
L	Distance between the centers of two bursts [m]
m_p	Mass of a particle [kg]
M	Surface particle concentration [$\mu\text{g}/\text{m}^2$] or [$\#/\text{m}^2$]
M_{or}	Deposited mass of particles onto the sample substrate [g]
M_f	Mass of the gravimetric filter [g]
n_i	Number of particles left on the surface
n_p	Number of occupants indoors
n_0	Initial number of particles on the surface
n_i	Number of particle on the surface after a centrifuge experiment
N_0	Particle surface number concentration in the ventilation duct [$\#/\text{m}^2$]
p_h	Gaussian distribution function
p	Vapor pressure [Pa]

p_{b1}	Aerosol penetration through bends in the ventilation duct for outdoor particles
p_{b2}	Aerosol penetration through bends in the ventilation duct for resuspended particles
p_{b3}	Aerosol penetration through bends in the ventilation duct for the particles in the recirculated air
p_c	Penetration coefficient of particles through building shell
P_c	Width of ceiling of ventilation duct [m]
P_f	Width of floor of ventilation duct [m]
p_{fi}	Inhalability parameter accounting for the real exposure to pathogens
p_{fs}	Fraction of pathogens survived
P_i	Infection probability
p_s	Saturated vapor pressure [Pa]
P_v	Cross sectional perimeter of ventilation duct [m]
P_w	Width of wall of ventilation duct [m]
ΔP	Laplace pressure [Pa]
P_h	Combined Gaussian distribution function
Q_s	Ventilation rate [m ³ /s]
r	Kelvin radius [m]
r'	Radius of a burst [m]
r_i	Fitting parameter accounting for the infectivity of pathogen and the pathogen-host interactions in the exponential dose response model
r_{n1}	Coefficient in power law function of normalized resuspension rate
r_{n2}	Exponent in power law function of normalized resuspension rate

r_1, r_2	Principal radii of curvature of toroidal geometry [m]
R	Resuspension rate [$\mu\text{g/s}$] or [$\#/s$]
R_p	Radius of particle [m]
R'	Radius of curvature [m]
R_g	Gas constant [$\text{J}/(\text{mol}\cdot\text{K})$]
R_r	Fraction of recirculated air from the exiting air
Re	Reynolds number
S_n	Newly occupied area [m^2]
S_f	Total area of flooring coupons [m^2]
S_o	Overlapping area [m^2]
S'_o	Total area that the new burst overlaps with the previous bursts [m^2]
S_r	Particle resuspension area [m^2]
S_v	Dose area of BW in the ventilation duct [m^2]
t	Time [s]
Δt	Time difference between AIPR and WIPR [s]
Δt_s	Sampling interval of aerosol spectrometer [s]
T	Period of occurrence of bursts [s]
T_e	Exposure period [s]
T'	Temperature [K]
T^+	Non-dimensional period of occurrence of bursts
u^+	Non-dimensional velocity
u_t^+	Non-dimensional overall velocity during the turbulent burst-sweep event
u'	RMS longitudinal fluctuating velocity [m/s]
u^*	Friction velocity [m/s]

u	Air flow velocity [m/s]
u_f	Function between f' and y
U_∞	Free stream velocity [m/s]
v'	RMS normal fluctuating velocity [m/s]
v_f	Inverse function of u
v_{df}	Particle deposition velocity onto floor [m/s]
v_{dw}	Particle deposition velocity onto wall [m/s]
v_{dc}	Particle deposition velocity onto ceiling [m/s]
v_{dfv}	Particle deposition velocity onto the floor of ventilation duct [m/s]
v_{dwv}	Particle deposition velocity onto the wall of ventilation duct [m/s]
v_{dcv}	Particle deposition velocity onto the ceiling of ventilation duct [m/s]
V	Volume of indoor space [m ³]
$\dot{V}$	Sampling rate of the aerosol spectrometer [m ³ /s]
V_c	Volume of the resuspension chamber [m ³]
V_d	Overall deposition velocity in the ventilation duct [m/s]
V_w	Molar volume of water [m ³ /mol]
w'	RMS spanwise fluctuating velocity [m/s]
x_1	Mean square roughness of surface [m]
x_2	Mean square roughness of particle [m]
x_{v1}	Ventilation duct length passed by the entering outdoor particles [m]
x_{v2}	Ventilation duct length passed by the resuspended particles [m]
x_{v3}	Ventilation duct length passed by the particles in the recirculated air [m]
X_1	Random variable representing the mean square roughness for surface
X_2	Random variable representing the mean square roughness for particle

γ_r	Sum of mean square roughnesses for surface and particle [m]
γ_h^+	Non-dimensional height from the surface
γ_h	Height from the surface [m]
Y	Random variable representing the sum of mean square roughnesses for surface and particle
z	Height scope influenced by meniscus [m]
z_u	Vertical distance from the surface [m]
z_{u0}	Aerodynamic roughness length [m]

Greek symbols

α	Shape parameter of gamma distribution
α_a	Air exchange rate [1/s]
α_i	Fitting parameter accounting for the infectivity of pathogen and the pathogen-host interactions in the beta-Poisson dose response model
β	Scale parameter of gamma distribution
β_b	Breathing rate of an occupant [m ³ /s]
β_p	Particle decay loss rate [1/s]
Γ	Gamma function
γ	Surface energy of adhesion [J/m ²]
γ_1	Surface energy of surface [J/m ²]
γ_2	Surface energy of particle [J/m ²]
γ_d	Decay rate of pathogen [1/s]
γ_w	Surface tension of water [N/m]

δ_0	Parameter defining symmetric rectangular distribution of roughness [m]
δ_1	Approach distance [m]
$\bar{\delta}_1$	Average approach distance of asperities [m]
δ_2	Stretching distance [m]
$\bar{\delta}_2$	Average stretching distance of asperities [m]
ϵ_i	Fitting parameter accounting for the infectivity of pathogen and the pathogen-host interactions in the beta-Poisson dose response model
η	Kinematic viscosity [m ² /s]
η_r	Removal efficiency of filter in the ventilation duct
θ	Contact angle
θ_1	Contact angle of surface
θ_2	Contact angle of particle
κ	Von Kármán constant
λ	Contact length scale [m]
λ'	Peak to peak distance [m]
$\bar{\lambda}$	Average peak to peak distance between asperities [m]
λ_a	Scan length scale [m]
λ_l	Longitudinal spacing of bursts [m]
λ_l^+	Non-dimensional longitudinal spacing of bursts
λ_s	Spanwise spacing of bursts [m]
λ_s^+	Non-dimensional spanwise spacing of bursts
Λ	Normalized resuspension rate [1/s]
μ	Dimensionless parameter for differentiating the ranges of validity for the JKR model and DMT model

μ_{adh}	Mean parameter of adhesion force distribution
μ_r	Mean of RMS roughness distribution
ν	Poisson ratio
ν_1	Poisson ratio of surface
ν_2	Poisson ratio of particle
Σ_1	Random variable representing the RMS roughness of surface
Σ_2	Random variable representing the RMS roughness of particle
σ	RMS roughness under the length scale λ [m]
σ_a	RMS roughness under the length scale λ_a [m]
σ_1	RMS roughness of surface [m]
σ_2	RMS roughness of particle [m]
σ_{adh}	Dispersion parameter of lognormal adhesion force distribution
σ_r	Standard deviation of RMS roughness distribution
ρ_a	Density of air [kg/m ³]
ρ_f	Density of fluid [kg/m ³]
ρ_p	Density of particle [kg/m ³]
τ_w	Shear stress [kg/(m·s ²)]
ω	Rotational speed [rpm]

Chapter 1 Introduction

1.1 Background

Historical outbreaks of infectious disease (e.g., the Black Death of 1347 – 1352 and the Influenza Pandemic of 1918) have ever caused massive civilian casualties. Despite the significant improvement of modern medicine and living standards, some of these diseases still impose great threat to the life of human being. For instance, there are an estimated 8.3 million new tuberculosis (TB) cases in 2000 [1] and it is estimated that there were more than 40,000 deaths annually in industrialized nations due to TB [2]. There are 1.5 million deaths from respiratory infections worldwide annually [3]. Meanwhile, newly emerging infectious diseases put further threat to humans due to the lacking of the relevant control and management knowledge by the time they break out. A typical example is the outbreak of severe acute respiratory syndrome (SARS) in Southern China during 2002 – 2003, which causes great panic in the public due to the high fatality rate of the disease [4].

The anthrax letter incidents of 2001 in the United States leading to 22 anthrax cases raise the additional concern about the spread of infection by bioterrorist attack. The bioterrorist attack by the intentional release of aerosolized biological weapons (BW) such as highly infectious viruses is characterized by being of relatively low costs and technical challenges, causing injury and death in strange and prolonged ways, and being of the potential to produce huge economic loss [5]. For example, the release of 50 kg anthrax spores upwind of a city of 500,000 people will cause approximated

95,000 deaths and 125,000 hospitalizations [6]. It is estimated that the post-attack cost would be as high as \$26.2 billion per 100,000 persons exposed to BW agents [7].

In order to minimize the loss of life and property in case of an outbreak or a bioterrorist attack, appropriate measures are needed to effectively control and manage the infection transmission. Risk assessment of infection transmission can serve as one of such measures, since it could contribute to preclude infection and handle post-epidemic or post-attack situation. For example, the risk assessment of potential bioterrorist attack will help civil engineering professionals design safer and cost-effective buildings against the attack [8]. The risk assessment could provide the decision-makers and public with instructive knowledge (e.g., the scope of infection outbreak, the efficiency of decontamination measures and personal protective equipment (PPE)) against the outbreak or bioterrorist attack. However, the prerequisite of risk assessment is pathogen exposure analysis, which further necessitates a clear understanding of airborne and surface pathogen concentrations [9].

People spend most of their time (70% – 90%) indoors [10, 11] and most of pathogens could not survive for long period of time outdoors due to the germicidal effect of sunlight [12]. As a result, it is important to develop the capability of analyzing indoor human exposure to pathogens and corresponding infection risk, which requires the accurate understanding of indoor particle (pathogen is treated to be a particle) dynamics. As one of important interactions between aerosol and surface indoors, particle resuspension is the process when the previously deposited particles are detached from the surface and become airborne again. This process serves to transfer particles on surface compartment to air compartment and thus can affect indoor

particle dynamics. Existing studies [13-18] show that the particle resuspension from indoor surfaces or ventilation ducts could lead to the significant increase of human exposure to particles indoors. In the case of infection transmission, the resuspension of pathogens could lead to the secondary infection risk via inhalation [19-21]. Actually, there have been a variety of studies [22, 23] [24-29] suggesting that infection could be transmitted by pathogen resuspension.

Particle resuspension is governed by the interaction between the detachment forces and adhesion forces. Since the detachment and adhesion forces are generally associated with the surrounding environmental conditions and physicochemical properties of the particle and surface, the resuspension process is influenced by a variety of factors (e.g., airflow velocity, particle size, surface roughness, surface energy of materials, walking rate etc.). Depending on the source of detachment forces, there are airflow-induced particle resuspension (AIPR) and human-activity-induced particle resuspension (HAIPR) related to indoor environment.

In the case of AIPR, hydrodynamic forces serve as the detachment forces, while van der Waals force and capillary force are the main adhesion forces between a surface and submicron-sized or micron-sized particles corresponding to pathogen exposure analysis. Turbulent flow always exists in indoor environments and ventilation ducts [30, 31]. The models of turbulent hydrodynamic forces experienced by spherical particles have been proposed by a great number of previous studies. On the other hand, the current capability of predicting particle-surface adhesion is still limited. Most of existing adhesion force models intend to predict the “mean” adhesion force between rough particles and surface and are limited to nanoscale roughness. This goes against

accurate modelling of the particle resuspension process, because (1) in a real indoor environment and ventilation duct, the roughnesses of both particles and surfaces will not be limited to nanoscale, but should actually be of a multi-roughness scale feature; (2) the adhesion force between particles and the surface generally follows a distribution rather than a single value due to the existence of surface roughness, meaning the adhesion force distribution should be applied for modelling particle resuspension. Hence, it is necessary to improve the current capability of modelling particle-surface adhesion force, in order to accurately modelling the particle resuspension process.

Despite the complication of AIPR, some essential characteristics underlying the process could be identified after examining the hydrodynamic detachment force, adhesion force and physical phenomena of the process. For example, turbulent bursts play an important role for particle resuspension as they can modify the hydrodynamic forces experienced by particles. The resuspendable particles will be depleted as the resuspension progresses, since the more lightly adhered particles will be firstly resuspended, leaving the more tightly adhered ones on the surface. The environmental relative humidity (RH) could affect the resuspension process via affecting the capillary force. These characteristics should be included during the development of a physically reasonable AIPR model.

Particle resuspension from ventilation duct is a major AIPR case relevant to indoor particle concentration. Especially, in the case of a ventilation system-targeted bioterrorist attack, BW agents may be deliberately dosed onto the duct surface when the ventilation system is off (usually at night, therefore more covert). Once the

ventilation system is turned on again, some of these dosed agents could be resuspended and transported into indoor environment, leading to mass contamination [32-35]. In order to control and manage this kind of attack, the knowledge of particle concentration dynamics in the ventilation duct with the occurrence of AIPR is needed for performing the corresponding indoor exposure analysis. A model of particle concentration dynamics in the ventilation considering AIPR could serve such a purpose.

Human activities that resuspend particles indoors include walking, vacuuming and bed folding, etc. Among these activities, walking is one of the most common ones capable of causing significant particle resuspension [36-39] and will be investigated in this work. In the case of walking-induced particle resuspension (WIPR), both hydrodynamic forces (due to high speed jet and large-scale ring vortex structures) and mechanical disturbances (e.g., impaction and vibration) contribute to resuspend particles. It is still difficult to theoretically model WIPR for the time being due to the great difficulty of modelling the detachment forces involved. An experimentally determined empirical model could be an alternative choice for quantifying WIPR. In this work, a series of experiments were conducted to quantify the resuspension rate of WIPR from various common flooring materials and an empirical resuspension rate model will be proposed by fitting a certain function to the experimental data.

The effect of AIPR and HWIRP could be substituted into two-compartment (air and surface compartment) mass balance models to develop the analytical models of indoor particle concentrations. Then, exposure analysis could be conducted in terms of such developed analytical models. The ultimate goal of this work, that is, the risk

assessment of infection transmission, could be achieved by integrating the exposure analysis into a dose response model. The impact of resuspension on infection transmission could be clearly identified based on the risk assessment scheme, which will generate insights over the control and management of infection transmission indoors.

Figure 1.1 The knowledge hierarchy of this work.

The knowledge hierarchy of this work is shown in Figure 1.1. The dash line encircled parts are the knowledge gaps to be filled by this study, while the solid line encircled parts are the knowledge available from existing literature. The ultimate goal (highlighted by yellow background in Figure 1.1) of this work is to develop a risk assessment scheme where the role of resuspension could be identified. Correspondingly, the objectives and scope of this work are presented as follows.

1.2 Objectives and scope

This work aims to investigate particle resuspension processes and their potential role in infection transmission and to develop the corresponding models. In order to achieve the objectives, the specific scope of this work is as follows.

(1) Models for AIPR and WIPR will be developed, respectively. The proposed new models will improve the current capability of quantifying resuspension processes. It will be achieved through several sub-scopes.

(a) A model of particle concentration dynamics in the ventilation duct with AIPR will be proposed (Chapter 3).

(b) Experiments will be conducted to investigate WIPR, based on which an empirical resuspension rate model of WIPR will be developed (Chapter 4).

(c) Particle-surface adhesion force models will be proposed (Chapter 7 and 8).

(d) Knowledge of turbulent flow related to particle resuspension will be compiled from literature (Chapter 2).

(e) A theoretical AIPR model will be proposed based on (c) and (d) (Chapter 9) which has the potential to be used in exposure modelling in the future.

(2) A risk assessment scheme for indoor infection transmission incorporating the effect of pathogen resuspension will be developed. The impact of resuspension on infection transmission could be clearly identified through the scheme. It will be achieved through several sub-scopes as well.

(f) The models from (a) and (b) will be substituted into two-compartment mass balance models to develop indoor particle concentration models, based on which exposure analysis will be performed (Chapter 2, Chapter 5 and Chapter 6).

- (g) The information on the biological and epidemiological aspect of pathogens and dose response model will be compiled from literature (Chapter 2).
- (h) A risk assessment scheme will be proposed by combining the exposure analysis model from (f) with the information from (g) (Chapter 6).

Chapter 2 Literature Review

2.1 Overview of indoor infection transmission modes and existing risk assessment schemes

2.1.1 Infection transmission modes

There are three major modes by which infection transmission could occur indoors, i.e., droplet, airborne and contact modes, respectively [40]. The droplet mode refers to the direct transfer of pathogen-laden expiratory particles of large size ($\sim >100\ \mu\text{m}$) from the infector to the susceptible people. This mode usually occurs over distances of no more than 1.5 meters, because these relatively large particles quickly settle out of the air. The airborne mode refers to the inhalation of pathogen-laden particles which are small enough to remain airborne for sufficiently long time and could be dispersed to long distances following the airflow. The airborne transmissible particles usually include droplet nuclei which are the product of droplet after evaporation, skin flakes shed from the skin of individuals heavily colonized with pathogens such as *staphylococci*, and aerosolized pathogens such as those from a bioterrorist attack. The contact mode refers to the direct contact with an infected person or indirect contact through an intermediate object such as fomite (microbes that settle onto surfaces or skin) with subsequent self-inoculation.

Deposition serves to reduce airborne pathogen concentration and thus the infection risk via the airborne mode. Actually, more than 70% by mass of the expiratory aerosols deposits on surfaces within a short time, instead of remaining airborne [41]. Some of these deposited pathogens could maintain their infectivity for extended

periods. As a result, the surfaces deposited with pathogens could serve as pathogen reservoirs for the infection transmission via the airborne mode, since they could be resuspended and subsequently inhaled by susceptible people. Existing studies have suggested that infection could be transmitted by pathogen resuspension. For example, Walter and Kundsinn [22] demonstrate that the floor of hospital could be a source of pathogens even after thorough cleaning. Kent [23] indicates that several tuberculosis epidemics in a US Navy ship could have been caused by pathogen resuspension, considering that new infections continuously occur even after the active disease have been removed from the ship. Barker and Jones [24] find that flushing a domestic toilet could disseminate micro-organisms such as *norovirus* into the air and lead to a potential infection risk via inhalation and swallowing. The incident that the carpet installers are infected by Norwalk-like virus 12 days after the end of an outbreak also implicates that the pathogen resuspension from the carpet could have led to the infection [25]. The study of Chen et al. [26] mentions that the resuspension of contaminated particles is able to enhance the cross-infection risk for dental healthcare workers (DHCWs) in dental clinics. The study of Goebes et al. [27] find that the significant increase of airborne *Aspergillus* concentration due to walking over carpet may result in invasive aspergillosis, a potentially fatal infection in immunocompromised people. The modelling by Price [28] manifests the resuspension of anthrax spores after a bioterrorist attack is a potential infection risk for residents. Recently, Nazaroff [29] indicates that the fomite on a heavily trafficked floor might become a secondary source of infectious particles due to human walking. On the whole, pathogen resuspension can impose potential exposure risk for residents and serve as a possible route for infection transmission. The capability of accurately quantifying the effect of resuspension on infection transmission contributes to

complete the understanding of transmission dynamics, which critically relates to the post-epidemic or post-attack response. Hence, it is necessary to take the impact of resuspension into consideration in order to develop a complete infection risk assessment scheme.

2.1.2 Existing risk assessment schemes

One of important steps towards well controlling infections is to set up reasonable risk assessment schemes. A great number of risk assessment schemes of infection transmission have been proposed in previous studies. For example, Nicas [42] develops a risk assessment scheme for assessing the occupational infection risk of airborne *M. tuberculosis*. Armstrong and Haas [43, 44] develop a scheme to assess the infection risk of legionnaire's disease with the dose response relationship established based on animal data. Atkinson and Wein [45] compare the infection risks of pandemic influenza via different transmission modes using their risk assessment scheme. The study of Kowalski et al. [46] investigates the infection risk in the case that BW agents are injected into the air-handling unit of a high-rise building. Based on a dose response model, Reshetin and Regens [47] propose a scheme to assess the infection risk of anthrax in a high-rise building after the intentional release of spores on the ground floor. Price et al. [48] develop a framework for evaluating the anthrax risk in buildings based on the steady state mass balance model. Hong and Gurian [49] devise a framework for estimating the risk for the case of indoor aerosolization of BW pathogens based on surface sampling of microorganisms. On the basis of the study of [49], Hong et al. [21] propose an integrated risk assessment scheme for the intentional

release of five Category A BW agents (*B. anthracis*, *Y. pestis*, *F. tularensis*, *Variola major* and *Lassa*) indoors.

Within the existing schemes, however, very few [21, 48] explore the possible infection risk from pathogen resuspension and constant resuspension parameters are generally assumed for analysis. This is caused by the lacking of data for resuspension processes. Hence, the knowledge about the influence of pathogen resuspension towards infection transmission is still limited for the time being, which obviously goes against the risk assessment-based control and management of infectious diseases. For analyzing indoor pathogen exposure and thus infection risk accurately, it is necessary to develop the capability of effectively modelling particle resuspension which is governed by the interaction between adhesion forces and detachment forces.

2.2 Adhesion force model

Adhesion force models will be applied for modeling AIPR in this work. For particles on a surface, there exist various types of adhesion forces between the particles and surface due to the intermolecular interactions. The adhesion forces mainly consist of van der Waals force, capillary force and electrostatic force. Under normal atmospheric conditions (e.g., room temperature and RH), the Boltzmann equilibrium charge state can be achieved for aerosol particles. With the average Boltzmann equilibrium charge, the electrostatic force between the particle smaller than hundreds of micrometers and the contacting surface could be two orders of magnitude smaller than the van der Waals force, according to the study of Zhou et al. [50] and Gady et al. [51]. In humid conditions, capillary force becomes significant and could even overtake the van der

Waals force if the RH is high enough. In the cases analyzed by Bowling [52], the capillary force could be almost one order of magnitude larger than the van der Waals force for particles of 0.1 to 100 μm in diameter. Furthermore, high humidity would also weaken electrostatic force due to the decrease of electrostatic potential [53], which further weakens the influences of electrostatic force compared to the van der Waals force and capillary force. In general, van der Waals force and capillary force will play a major role in the adhesion force between a small particle and surface under normal atmospheric conditions. Hence, the capability to predict van der Waals force and capillary force is the key to accurate prediction of particle-surface adhesion and thus AIPR. It should be noted that although the dominant role of van der Waals force and capillary force over electrostatic force could approximately hold for AIPR, the effect of electrostatic force on WIPR could not be neglected due to the triboelectric charging effect from walking. However, WIPR will be explored by a series of walking experiments rather than theoretical modeling in this work, the effect of electrostatic force on WIPR will not be explored in detail.

2.2.1 Mean adhesion force model

Over the past decades, a great number of mean adhesion force models have been proposed for the van der Waals force and capillary force, respectively, but these models suffer from different limitations. Johnson et al. [54] and Derjaguin et al. [55] derive the JKR (Johnson-Kendall-Roberts) and DMT (Derjaguin-Muller-Toporov) models, respectively, with the consideration of elastic deformation. Both of them could be used to predict particle-surface van der Waals force based on the surface energy and particle size and are subject to different ranges of validity. However, both

JKR and DMT models are only suitable for predicting the van der Waals force between a smooth particle and surface. Rumpf [56] develops a model predicting the van der Waals force between a smooth particle and a rough surface by treating the surface roughness with the spherical asperity radius. Later on, Rabinovich et al. [57, 58] introduce the model with the root mean square (RMS) roughness and the distance between spherical asperities to predict the van der Waals force between a smooth particle and a rough surface:

$$F_v = \frac{A_h R_p}{6D^2} \left[\frac{1}{1+51.84R_p \frac{\sigma_1}{\bar{\lambda}^2}} + \frac{1}{\left(1+\frac{1.817\sigma_1}{D}\right)^2} \right], \quad (2.1)$$

where A_h is the Hamaker constant, $\bar{\lambda}$ is the average peak-to-peak distance between asperities, R_p is the particle radius, σ_1 is the RMS roughness of surface and $D \approx 0.3$ nm is the equilibrium distance between the particle and surface. All these models [56-58] are only applicable for the surfaces with nanoscale roughness, whereas the roughness of surfaces such as that in an indoor environment might not be limited to nanoscale but should be of multi-scale feature, which necessitates the determination of the effective roughness relevant to the adhesion forces. Furthermore, the application of these models is also limited by the failure of considering the effect of particle roughness.

For the capillary force, Orr et al. [59] and Pakarinen et al. [60] developed the models for smooth particles and surfaces, which would also overestimate the capillary force between rough particles and surfaces. Their models predict that the capillary force is independent of RH, which is obviously inconsistent with the experimental observations that capillary force increases with RH [61, 62]. Rabinovich et al. [63] derive a model for the capillary force between a smooth particle and a rough surface:

$$F_c = 4\pi\gamma_w R_p c \left[1 - \frac{H_c}{2rc}\right], \quad (2.2)$$

where γ_w is the surface tension of water, c is the factor related to contact angles of the particle and surface, r is the Kelvin radius and $H_c = 1.817\sigma_1$ is the separation distance between the average surface plane and particle caused by surface roughness. This model is applicable only if $H_c \leq 2rc$, causing the model to be applicable for nanometer or even sub-nanometer scale roughness only. In addition, this model treats the surface roughness as a single asperity, which might oversimplify the surface morphology. Because real surfaces do not have single spherical asperity in roughness but a variety of asperities (a distribution of roughness across different length scales). Recently, Butt [64] develops a model for calculating the capillary force between a rough particle and surface. Theoretically, the general model of Butt [64] is suitable for any kind of statistical surface roughness distribution. However, the general model itself cannot be directly applied for predicting capillary force until it is further extended to consider a roughness distribution. For the simplicity and illustrative purpose, the general model has been extended to consider a symmetric rectangular distribution in his original paper as

$$F_c = \begin{cases} \frac{\pi z^3 R_p \gamma_w}{3\delta_0^2 r} & 0 \leq z \leq \delta_0 \\ \frac{\pi R_p \gamma_w}{3\delta_0^2 r} [z^3 - 2(z - \delta_0)^3] & \delta_0 \leq z \leq 2\delta_0 \\ \frac{2\pi \gamma_w}{r} [R_p(z - \delta_0) - \frac{z^2 - 2z\delta_0}{2}] & 2\delta_0 \leq z \leq H_{\max} \end{cases}, \quad (2.3)$$

where $z = 2cr - D$, δ_0 is the roughness parameter defining the symmetric rectangular distribution and $H_{\max} = 2R_p$ is the maximum separation distance available for meniscus formation. The use of symmetric rectangular distribution leads to an obvious deficiency in predicting the adhesion force on real surfaces whose roughness

generally follows the Gaussian distribution [65, 66]. Meanwhile, the same as the above models, this model overlooks the multiple-scales nature of surface roughness.

Apart from the inherent limitations as discussed above, the application of the mean adhesion force models is also limited due to the fact that the actual adhesion force between particles and a surface generally follows a distribution rather than a single value [50, 67-77]. Therefore, solely understanding the mean adhesion force is not enough for accurate depiction of the actual particle-surface adhesion relevant phenomena (e.g., particle resuspension).

2.2.2 Adhesion force distribution model

Towards understanding adhesion force distribution, despite significant experimental effort has been taken [50, 67-77], few models have been proposed for the time being. Until recently, Prokopovich et al. [73, 74] propose a method for modeling the van der Waals force distribution by rendering a real surface with a number of randomly generated asperities. However, this method is specifically developed to model the van der Waals force distribution, which limits its application for the cases where the capillary force is also significant or even dominant. Therefore, the current capability of modeling adhesion force distribution is still limited, while the adhesion relevant processes are actually affected by adhesion force distributions rather than mean values.

2.3 Hydrodynamic force

2.3.1 Airflow velocity profile

Generally, the size of respirable particles as considered in this work is less than $10\text{ }\mu\text{m}$ [78], which is much smaller than the thickness of the viscous sublayer (several hundred micrometers) in the turbulent boundary layer. This means that these particles will submerge into the viscous sublayer where the relationship between the mean non-dimensional velocity u^+ and the non-dimensional height y_h^+ [79] is

$$u^+ = y_h^+, \quad (2.4)$$

where $u^+ = u/u^*$ with $u^* = (\tau_w/\rho_f)^{1/2}$ as the friction velocity. τ_w is the wall shear stress and ρ_f is the density of fluid. $y_h^+ = \frac{y_h u^*}{\eta}$ with η as the kinematic viscosity.

However, the viscous sublayer is anything but laminar [80]. Existing studies [81, 82] have shown that the viscous sublayer is continually erupting with turbulent bursts which penetrate deep into the wall region and lead to an unsteady viscous sublayer. The turbulent bursts are distributed fairly uniformly with a certain non-dimensional spanwise and longitudinal spacings λ_s^+ and λ_l^+ , and occur with a certain non-dimensional period T^+ [82-88]. A summary of the existing data about non-dimensional spanwise spacing λ_s^+ , longitudinal spacing λ_l^+ , and period T^+ is given by Table 2.1. In the case of turbulent bursts, the airflow streaks will be formed in the viscous sublayer and the airflow velocity will be modified [83]. The occurrence of turbulent bursts can be modeled based on the spatial and temporal parameters and the modified instantaneous velocity.

Table 2.1 Non-dimensional streamwise and spanwise spacings and period of turbulent bursts

Reference	λ_l^+	λ_s^+	T^+
-----------	---------------	---------------	-------

Blackwelder and Haritonidis [86]	—	—	300
Lu and Willmarth [89]	—	—	80
Morrison et al. [85]	630	135	75 – 80
Kim et al. [84]	—	60 – 130	88 – 106
Kline et al. [83]	—	100	103
Rao et al. [87]	—	—	72

According to the study of Ziskind [90], any velocity component within the sublayer depends on the non-dimensional distance y_h^+ , and the RMS longitudinal, normal and spanwise fluctuating velocities can be expressed as

$$\begin{aligned}
u' &= u^* f_1(y_h^+) \\
v' &= u^* f_3(y_h^+) \quad \text{and} \\
w' &= u^* f_2(y_h^+).
\end{aligned} \tag{2.5}$$

Given the condition that u' , v' , w' and the gradient of v' tend to be zero when approaching the wall, the Taylor-series expansions of $f_1(y_h^+)$, $f_3(y_h^+)$ and $f_2(y_h^+)$ lead to

$$\begin{aligned}
f_1(y_h^+) &= a_{y1} y_h^+ + b_{y1} y_h^{+2} + \dots \\
f_3(y_h^+) &= a_{y3} y_h^{+2} + b_{y3} y_h^{+3} + \dots \quad \text{and} \\
f_2(y_h^+) &= a_{y2} y_h^+ + b_{y2} y_h^{+2} + \dots
\end{aligned} \tag{2.6}$$

The coefficients of the first order terms, a_{y1} , a_{y2} and a_{y3} could be determined by experimental or numerical studies with the higher order terms neglected. The longitudinal and spanwise fluctuating velocities have been measured by Alfredsson et al. [91] using hot-film probes as $u' = 0.40u^* y_h^+$ and $v' = 0.20u^* y_h^+$, respectively. The normal fluctuating velocity [92-94] is significantly smaller than the longitudinal and spanwise ones and thus negligible. The instantaneous longitudinal and spanwise

velocities are resultant by the sum of the respective mean velocity and fluctuating velocity:

$$\begin{aligned} u^+ &= 1.40y_h^+ \text{ and} \\ v^+ &= 0.2y_h^+. \end{aligned} \quad (2.7)$$

Hence, the relationship between the non-dimensional overall velocity, $u_t^+ = \sqrt{u^{+2} + v^{+2}}$ and the non-dimensional height y_h^+ during a turbulent burst-sweep event is

$$u_t^+ = 1.41y_h^+. \quad (2.8)$$

2.3.2 Models of hydrodynamic forces

Depending on the particle size, the lift force is calculated using the models from [95] or [96]

$$F_L^+ = \begin{cases} 0.58 \left(\frac{du^+}{dy^+} \right)^2 (d_p^+)^4, & d_p^+ \leq 3.6 \\ (20.90 \pm 1.57)(d_p^+/2)^{(2.31 \pm 0.02)}, & 3.6 < d_p^+ < 140 \end{cases} \quad (2.9)$$

where $F_L^+ = \frac{F_L}{\eta^2 \rho_f}$ is the non-dimensional lift force. $d_p^+ = \frac{d_p u^*}{\eta}$ is the non-dimensional particle diameter. The drag force model has been derived by O'Neill [97] as

$$F_D^+ = 1.5\pi \frac{du^+}{dy^+} (d_p^+)^2 f_d, \quad (2.10)$$

where $F_D^+ = \frac{F_D}{\eta^2 \rho_f}$ is the non-dimensional drag force. $f_d = 1.7$ is a correction to the Stokes drag force accounting for the wall effect.

2.4 Model of AIPR

Generally, AIPR models can be categorized into two groups [98]. The first group refers to the theoretical models that describe the resuspension process in terms of micro-scale mechanisms. The second group consists of the macroscopic, empirical models that are derived by regression analysis or dimensional analysis of data from wind tunnel experiments.

2.4.1 Theoretical model

There are two types of theoretical AIPR model which are based on force balance and potential energy balance, respectively. The models based on force balance assume that particle resuspension will occur if the hydrodynamic forces (moments) exceeds the adhesion forces (moments). The models based on potential energy balance assume that particle resuspension will occur if enough turbulent energy is gained by the particle to overcome the adhesive potential well.

2.4.1.1 Models based on force balance

As described above, turbulent bursts play an important role in particle resuspension in turbulent flow. This has been considered by some AIPR models based on force balance. The first attempt of including turbulent bursts to model the resuspension process is taken by Cleaver and Yates [99]. They assume that if a portion of surface is exposed to a turbulent burst, a 0.01 fraction of particles lying beneath the burst will be resuspended. Without the occurrence of bursts, a particle will be detached when the hydrodynamic lift force is larger than the adhesion force. However, it is lacking of mechanistic explanation for the assumed fraction of 0.01.

In the study of Braaten et al. [100], Monte Carlo simulation is conducted to model AIPR by assuming that both the adhesion force and hydrodynamic force followed certain distributions. The adhesion force distribution is obtained by the centrifuge method, while the hydrodynamic force distribution is determined by backward fitting the resuspension data. However, the model does not consider about the random spatial distribution of bursts in a certain area. The backward fitting of hydrodynamic force distribution limits the practical application of the model.

Matsusaka and Masuda [101] introduce the generation probability of turbulent bursts and the lognormal adhesion force distribution into their AIPR model. Their model does not take the spatial and temporal distribution of turbulent bursts and velocity fluctuation into consideration. The parameters for the adhesion force distribution are obtained by backward fitting the experimental data, which also limits the application of the model.

Wen and Kasper [102] develop a AIPR model by analogizing the resuspension process to the process of molecular desorption from inhomogeneous surface. In the model, the amount of resuspended particles per unit time is exponentially dependent on the ratio of the adhesion force to the removal force. Despite realizing the existence of adhesion force distribution, they introduce the unusual uniform distribution into the model, which limits the practical application of the model. Furthermore, the model of Wen and Kasper [102] does not explicitly take the effect of turbulent bursts into consideration.

Zhu et al. [103] extend the model of Cleaver and Yates (1973) to evaluate the AIPR in ventilation ducts. However, their model fails to consider about the adhesion force distribution and the depletion of resuspendable particles. This disables their model to predict the decline trend of normalized resuspension rate (the fraction of particles resuspended from the surface per unit time) with respect to time which has been widely observed [32, 104, 105].

Recently, Goldasteh et al. [106-108] model the particle resuspension process under turbulent flow with the consideration of surface roughness. However, their models generally consider the van der Waals force with a model that is limited to surfaces with nano-scale roughness and do not explicitly consider about the effect of adhesion force distribution. Moreover, during the model validation, the parameters determining the adhesion force were obtained by backward fitting of the experimental resuspension data used for validation, suggesting that the practical application of their model may be limited as well.

2.4.1.2 Models based on potential energy balance

The concept of potential energy balance is firstly introduced by Reeks et al. [109] in their so-called RRH model. It is regarded in the model that the mean lift force modifies the shape and height of the adhesive potential well, while the fluctuating lift force makes the particle to deform in a random oscillatory fashion (Figure 2.1). The probability that a particle is detached from a surface per unit time is defined. This probability is directly proportional to the bursting frequency and exponentially dependent on the ratio of the accumulated average potential energy from turbulent

flow to the height of adhesive well. The adhesion force is considered by the JKR model [54] together with an assumed roughness distribution. It is found that the variation of normalized resuspension rate, $\Lambda(t)$ is clearly differentiated in terms of two periods: (1) the short ‘initial’ resuspension period ($t \leq 10^{-2}s$) when the normalized resuspension rate is very high; (2) the longer resuspension period ($10^{-2}s \leq t \leq 10^5s$) when the normalized resuspension rate varies almost inversely with respect to time, that is, $\Lambda(t) \sim t^{-1}$. Lazaridis et al. [110] modify the RRH model [109] by calculating the particle-surface adhesion force from a microscopic model based on the Lennard-Jones intermolecular potential.

Vainshtein et al. [111] employ the above potential well concept and introduce a tangential pull-off force needed to resuspend a particle in their so-called VZFG model. Corresponding to the tangential pull-off force, the model assumes that the particle performed streamwise oscillations due to the turbulent drag force instead of the vertical oscillations due to the turbulent lift force in the RRH model [109] as shown in Figure 2.1.

Recently, Reeks and Hall [112] develop the so-called rock’n roll model that have a similar principle as the RRH model [109]. But the rock’n roll model assumes that the particle oscillates around a pivot rather than oscillates vertically as considered in the RRH model (Figure 2.1), which leads a higher normalized resuspension rate to be predicted than the RRH model.

Figure 2.1 Particle oscillations in different energy balance-based AIPR models.

In the above models based on potential energy balance, the spatial distribution and the depletion of resuspendable particles on the surface are not considered, and the applied adhesion force distribution is implicitly determined by backward fitting the experimental data. This means that the forward prediction from these models will be still limited due to the lacking of knowledge about the adhesion force distribution. Last but not least, all the AIPR models (force balance and potential energy balance) are not able to predict the effect of RH in AIPR, which prevents the practical application of these models for the cases where the capillary force between the particle and surface is significant.

2.4.2 Empirical model

Empirical resuspension models have been developed by fitting an exponential law function or a power law function to the experimentally determined resuspension factor (the ratio of airborne particle concentration to surface particle concentration) or normalized resuspension rate. A number of such models [113-115] have been developed to describe the atmospheric resuspension of radionuclide. But these models [113-115] are based on the outdoor radionuclide resuspension data for the period from months to years and thus more suitable for predicting the resuspension process under a large time scale. Realizing the need to have a resuspension model applicable for

shorter time scales (several hours and days), Loosmore [116] derives the empirical resuspension models (emp1 and emp3) based on the regression analysis of the existing data from wind tunnel experiments:

$$\Lambda = 0.42 \frac{u^{*2.13} d_p^{0.17}}{t^{0.92} \sigma_1^{0.32} \rho_p^{0.76}} \quad (\text{emp1}) \quad (2.11)$$

$$\Lambda = 0.01 \frac{u^{*1.43}}{t^{1.03}} \quad (\text{emp3}) \quad (2.12)$$

where t is the time, σ_1 is the surface roughness and ρ_p is the density of particle. Recently, Kim et al. [98] derives three empirical models based on the dimensional analysis (Buckingham π theorem) of the data from wind tunnel experiments. The models of Kim et al. [98] considere more parameters, such as air density and Hamaker constant, than the models of Loosmore [116] as shown by one of the three models (Model II-A):

$$\begin{aligned} \frac{\Lambda d_p}{u^*} = & \\ & 8.521 \times \\ & 10^{-3} \left(\frac{\rho_p}{\rho_a} \right)^{-0.3028} \left(\frac{u^* t}{d_p} \right)^{-1.0135} \left(\frac{\sigma_1}{d_p} \right)^{-0.3269} \left(\frac{A_h}{d_p^3 u^{*2} \rho_a} \right)^{-0.2961}, \end{aligned} \quad (2.13)$$

(Model II-A)

where ρ_a is the density of air.

2.5 WIPR

Human walking has been found to be one of the important mechanisms of resuspending particles indoors, which could be a significant source of inhalation exposure to particles [13, 15, 18, 117-121]. Thatcher and Layton [13] find that walking into and out of a room could double the airborne mass concentration of

coarse particles ($>5\ \mu\text{m}$) in the room. The study of Qian et al. [119] shows that the average mass concentration of PM_{10} (particulate matters of sizes $\leq 10\ \mu\text{m}$) is 2.5 times as high as the background level with the occurrence of WIPR.

WIPR is caused by the high speed flow with large-scale vortex structures and the mechanical contact between the feet and floor [122-124]. Correspondingly, WIPR is affected by a variety of factors such as walking mode, walking speed, flooring material, particle size, RH, etc. For instance, the mass of particles resuspended from a carpet by walking with rotation is found to be 2 times larger than that by walking without rotation [117]. The resuspended PM_{10} by walking are dominated by particles larger than $2.5\ \mu\text{m}$ in terms of mass concentration [118]. The study of Qian and Ferro [18] show that the normalized resuspension rate of walking on the hard floor (e.g., wood) is lower than walking on the carpet for $1.0 - 10\ \mu\text{m}$ particles. The study of Tian et al. [125] also finds that the resuspension from carpet is more significant than from hard floor for $3.0 - 10\ \mu\text{m}$ particles. Hence, WIPR is highly variable depending on the characteristics of walking and environment. In fact, the measured normalized resuspension rate for WIPR ranges from $10^{-5} - 10^{-2}\ \text{hr}^{-1}$ for $0.8 - 10\ \mu\text{m}$ particles.

The current understanding of WIPR is still limited. The effects of some factors such as walking rate, RH and mechanisms on WIPR have been rarely explored. Furthermore, existing resuspension rate data are generally obtained based on the assumption that the resuspension rate was constant during walking. Physically, however, the resuspension rate of WIPR will become smaller, since more and more particles are depleted from the surface, which has been referred as the “harvesting effect” in [119]. Therefore, more studies are needed to explore resuspension rate

dynamics which is critical for accurately modelling indoor particle dynamics and thus particle exposure involved with WIPR.

2.6 Indoor particle dynamics

In order to study the role of resuspension in infection transmission indoors, it is necessary to know how this process could affect indoor particle dynamics, which can be accomplished by solving the two-compartment (air and surface compartment, respectively) mass balance models [126-128].

2.6.1 Two-compartment mass balance models

The factors which affect indoor particle concentration include direct emissions from indoor sources, ventilation, penetration, deposition and resuspension, etc [129]. The influence of these factors towards indoor particle concentration could be considered by the two-compartment mass balance models:

$$\frac{dC_i}{dt} = a_1 C_o + a_2 C_{ov} - b C_i + \frac{R}{V} + \frac{E}{V} \quad (2.14)$$

$$\frac{dM}{dt} = C_i v_{df} - \frac{R}{S_r} \quad (2.15)$$

under the initial condition of $C_i(0)$ and $M(0)$. Eq. (2.14) and Eq. (2.15) account for the air and surface compartment, respectively. C_i and C_o are the indoor and outdoor airborne particle concentrations, respectively. C_{ov} is the airborne particle concentration in the ventilation duct due to the AIPR inside. M is the indoor particle concentration on the surface where resuspension occurs. V is the volume of indoor space. R is the resuspension rate of WIPR. v_{df} is the particle deposition velocity onto the floor. E is the indoor emission sources besides WIPR. S_r is the particle

resuspension area. According to the study of Thatcher and Layton [13], the resuspension area is defined as the area of floor that walking may reach during a activity period, which is applied in Eq. (2.14) and Eq. (2.15). It should be noted that this definition may not be accurate for describing actual resuspension areas by walking in some real cases. Hence, applying this definition may affect Eq. (2.14) and Eq. (2.15)-based model prediction. Whenever the actual resuspension area is known, it should be applied for the model prediction in Eq. (2.14) and Eq. (2.15). a_1 is the entrance rate of outdoor particles. a_2 is the entrance rate of resuspended particles from the ventilation duct. b is the loss rate of indoor particles. a_1 , a_2 and b are ventilation system dependent (i.e., mechanical ventilation and natural ventilation).

Figure 2.2 A schematic diagram of indoor particle dynamics for mechanical ventilation.

In the case of mechanical ventilation (Figure 2.2), $a_1 = (1 - R_r)(1 - \eta_r)p_{b1}d_{v1}\alpha_a$. α_a is the air exchange rate. R_r is the fraction of recirculated air from the exiting air. η_r is the removal efficiency of filter in the ventilation duct, which depends on the particle size and the type of filter. η_r can be obtained from the study of Riley et al. [130] for

some commonly used commercial filters such as 40% and 85% ASHRAE filters. p_{b1} is the aerosol penetration through bends in the ventilation duct for outdoor particles and could be estimated according to the theory of McFarland et al. [131]. d_{v1} is the parameter accounting for the effect of particle deposition in the ventilation duct and is calculated by $d_{v1} = e^{-\frac{(v_{dfv}P_f + v_{dww}P_w + v_{dcv}P_c)x_{v1}}{(1-R_r)Q_s}}$. v_{dfv} , v_{dww} and v_{dcv} are the deposition velocities of particles onto the floor, wall and ceiling of ventilation duct, respectively, which could be estimated based on the study by Sippola and Nazaroff [132] who have modeled the deposition loss of particles in ventilation ducts. P_f , P_w and P_c are the width of floor, wall and ceiling of ventilation duct, respectively. x_{v1} is the ventilation duct length passed by the entering outdoor particles. $Q_s = \alpha_a V$ is the ventilation rate. $a_2 = (1 - R_r)(1 - \eta_r)p_{b2}d_{v2}\alpha_a$. p_{b2} is the aerosol penetration through bends for resuspended particles in the ventilation duct. $d_{v2} = e^{-\frac{(v_{dfv}P_f + v_{dww}P_w + v_{dcv}P_c)x_{v2}}{(1-R_r)Q_s}}$. x_{v2} is the ventilation duct length passed by the resuspended particles in the ventilation duct. $b = \alpha_a - R_r d_{v3}(1 - \eta_r)p_{b3}\alpha_a + \frac{(v_{df}A_f + v_{dw}A_w + v_{dc}A_c)}{V} + \frac{\beta_b n_p}{V}$. v_{df} , v_{dw} and v_{dc} are the particle deposition velocities onto the indoor floor, wall and ceiling, respectively and can be estimated based on the model of Lai and Nazaroff [30] or experimental data [133]. A_f , A_w and A_c are the areas of indoor floor, wall and ceiling, respectively. β_b is the breathing rate of occupant. n_p is the number of occupants. $d_{v3} = e^{-\frac{(v_{dfv}P_f + v_{dww}P_w + v_{dcv}P_c)x_{v3}}{R_r Q_s}}$ accounts for the effect of particle deposition in the ventilation duct for the particles in the recirculated air. x_{v3} is the duct length passed by the recirculated air. p_{b3} is the aerosol penetration through bends in the ventilation duct for the particles in the recirculated air.

Figure 2.3 A schematic diagram of indoor particle dynamics for natural ventilation.

In the case of natural ventilation (Figure 2.3), $a_1 = p_c \alpha_a$. p_c is the penetration coefficient which ranges from 0 to 1, depending on the factors such as particle size and building conditions. Penetration coefficient could be estimated based on existing size-resolved experimental data [134-137]. $a_2 = 0$. $b = \alpha_a + \frac{(v_{df}A_f + v_{dw}A_w + v_{dc}A_c)}{V} + \frac{\beta_b n_p}{V}$. In Eq. (2.14) and Eq. (2.15), the particle coagulation and condensation are not taken into consideration. Wherever the effect of coagulation or condensation becomes significant (e.g., extremely high airborne particle concentration such as more than $1 \times 10^{10} \text{ \#}/\text{m}^3$ [138]), the model needs to be modified to account for the effect. The parameters are corresponding to the particles within a certain size bin in Eq. (2.14) and Eq. (2.15), which allows the particle size distribution to be considered implicitly.

It should be noted that pure AIPR from indoor surfaces is not considered in the above models (Eq. (2.14) and Eq. (2.15)). This is because pure AIPR indoors is generally negligible for normal indoor environment as the explanation follows. Previous studies [139-141] observe that the threshold friction velocity below which particle resuspension could not occur ranges from 0.1 to 0.3 m/s for particles up to several tens of micrometers. Meanwhile, the threshold friction velocity is larger for smaller

particles [90]. Therefore, considering that the representative friction velocity indoors ranges from 0.01 to 0.03 m/s [30], the pure AIPR indoors could hardly occur for exposure analysis-related particles which are generally smaller than 10 μm .

2.6.1.1 Direct emission sources

For general particulate matters (PM), indoor emission sources include cooking, tobacco smoking, and household appliances, etc. Relevant to pathogens considered in this work, indoor emission sources mainly include human expiratory activities (e.g., breathing, speaking, coughing, sneezing) [42, 142, 143] and pathogen aerosolization such as that during a bioterrorist attack [19, 46, 47, 144].

The size and number of particles emitted per expiratory activity have been reported by previous studies [145-150]. However, there is significant inconsistency in the reported data. For instance, [145, 146] report that the expelled particles by coughing are mainly in the size range of super-micrometer, while [148] shows that 80% – 90% of particles from coughing are smaller than 1 μm . [150] reports that the particles from coughing and talking predominantly range from 50 – 75 μm , while the study by [149] observes a size range of 4 – 8 μm . [146] shows that a sneeze produces around 40,000 particles and a cough produces a few hundreds of particles. [145] shows that about 1×10^6 and 5×10^3 particles are produced per sneeze and cough, respectively. Louden and Roberts [147], and Papineni and Rosenthal [148] find that the average number of particles emitted per sneeze and cough is 470 and 420, respectively. Although there is no definite conclusion over the size and number of particles expelled per expiratory

activity, sneezing will generally produce a larger number of particles and have a lower frequency compared to coughing, breathing and talking.

Aerosolization of BW agents such as that during a bioterrorist attack also serves as a potential emission source indoors. An typical example of this kind of emission is the 2001 anthrax letter incidence where the *Bacillus anthracis* spores are aerosolized during opening the spores-contained envelopes, which leads to 22 anthrax cases and 5 deaths [5]. [47] find that the aerosolization of even a relatively small volume of anthrax spore has the potential to distribute throughout a building within a short period of time. The study of [21] shows that the intentional aerosolization of five Category A BW agents indoors will lead to a significant inhalational risk. The study of Price et al. [48] quantifies the infection risk in the case of a bioterrorist attack aerosolizing BW agents indoors. Recently, [49] develops a practical sampling standard for evaluating the infection risk after the aerosolization of BW agents indoors.

2.6.1.2 Ventilation

Ventilation serves to refresh indoor air with outdoor air. Generally, the viable pathogens from outdoor air could be negligible [151], because outdoor airborne microbes will quickly die off due to the strong inactivation factors, such as sunlight, oxygenation and desiccation. In this case, the ventilation will contribute to dilute the indoor pathogen concentration according to the mass conservation of air indoors [152]. However, in the case of a bioterrorist attack that releases hardy BW agents (e.g., *B. anthracis*) outdoors, the impact of outdoor pathogen concentration has to be taken

into consideration for modelling indoor particle dynamics. Furthermore, if BW pathogens are dosed into ventilation ducts, ventilation will intend to bring pathogens into indoor environment. The United States government has warned that the ventilation systems of buildings are an ideal target for bioterrorism [35]. There is evidence showing that terrorists have gained some training about injecting harmful agents towards the air intake of a building, according to the report of Kean [153]. The bioterrorist attack via a ventilation duct system can be accomplished by two ways. Firstly, terrorists could deliberately place BW agents onto the duct surface when the ventilation system is off. Some of these agents could be resuspended and transported into indoor environment once the ventilation system is turned on, leading to mass contamination [32-34]. Secondly, it is possible that BW agents are directly injected into the duct when the ventilation system is running. Some of these injected agents will be instantly transported into indoor environment along with the airflow, causing mass contamination.

2.6.1.3 Deposition

Indoor particle deposition can be caused by advection, molecular and turbulent diffusion, thermophoresis and external forces such as gravitation and electrostatic attraction. Molecular and turbulent diffusion are significant for the particles smaller than 0.1 μm , while gravitation settling becomes significant for particles larger than 1 μm [13, 133]. Thermophoretic deposition is significant for small particles in the presence of a modest temperature gradient, while electrostatic deposition occurs if a charged particle stays within an imposed field or beside a solid wall [154]. According to the mass balance model (Eq. (2.14)), the airborne particle concentration will

exponentially decay as time in a well-mixed and air-tight enclosure if there are no other sources and sinks except for deposition. The deposition parameters (e.g., particle decay rate loss coefficient and deposition velocity) could be evaluated by fitting the exponential law to the temporal concentration variation measured. Existing data of deposition parameters generally follow a V-shape with respect to the particle diameter [155]: larger particles and smaller particles have larger loss coefficients than those particles of intermediate sizes ($0.1 - 1 \mu\text{m}$).

2.7 Biological aspect of pathogen

In order to evaluate the infection risk for a certain pathogen, it is necessary to know the persistence and infective dose of the pathogen. Pathogen persistence affects the number of viable pathogens inhaled, while the infective dose is directly related to the infection probability after inhaling a certain amount of viable pathogens.

2.7.1 Persistence of pathogen

The persistence of pathogens depends on various factors, such as pathogen type, surface type, RH, temperature, UV radiation, with or without anti-pathogen chemical. There is no complete information about the effects of these factors on the survivability of pathogens for the time being. However, existing data support that pathogens are able to survive from several hours to weeks under normal indoor conditions. For instance, it is observed that the enveloped enteric viruses (e.g., *astrovirus*) could survive on indoor surfaces from several hours to several days, while the non-enveloped viruses (e.g., *rotavirus*) are able to maintain infectious at least 2 months

[156]. The *poliomyelitis virus*, *echovirus* and *coxsackievirus* could remain infectious from 2 to more than 12 days on the surface of household objects [157]. Brady et al. [158] find that human parainfluenza viruses (hPIVs) 1, 3, and 4a could persist for up to 10 hrs on non-absorptive surfaces (e.g., stainless steel, laminated plastic and skin) and up to 4 hrs on absorptive surfaces (e.g., hospital gown, facial tissue and laboratory coat). Both influenza A and B virus are able to survive 24 – 48 hrs on stainless steel and plastic and more than 12 hrs on cloth, paper and tissues [159]. Norwalk-like virus causing gastroenteritis is able to survive on carpets for more than 12 days [25]. Small pox, a particularly dangerous BW agent, is able to survive in the environment for weeks [160]. The study of Hong et al. [21] summarizes the persistence of five Category A BW agents and finds that they are able to survive in the indoor environment from several hours to months. The long-term persistence of pathogens reinforces that pathogen resuspension is a possible route for infection transmission. The persistence of pathogens is generally described by the exponential function [161]:

$$p_{fs} = e^{-\gamma_d t} \quad (2.16)$$

where p_{fs} is the fraction of pathogens survived and γ_d is the decay rate of pathogen.

2.7.2 Infective dose

Whether a susceptible person will get infected or not is related to the amount of pathogens inhaled. A susceptible person will get infected only if enough number of viable pathogens reaches the target cell and starts the multiplication. That is, there is an infective dose for each type of pathogen. The infective dose of a certain pathogen is influenced by a number of factors such as the age of host, the health status of host, the host's previous exposure to the pathogen, the pathogen type, the infection site, the

exposure route [162]. Correspondingly, the infective dose of a certain pathogen will not be a fixed value but will be variable. Hence, the infective dose is generally defined in terms of probability. Specifically, the median human infective dose (HID50) is defined as the pathogen concentration required to infect 50% of the population and could be estimated based on dose response data [163]. For example, the HID50s of influenza are 0.6 – 3 TCID50 and 127 – 320 TCID50, when the virus is inhaled via the airborne route and intranasal droplet route, respectively [164]. TCID50 (median tissue culture infective dose) is the amount of pathogens that will produce pathological change in 50% inoculated cell cultures. Besides 50%, other probability could be used to define the corresponding infective dose.

2.8 Risk assessment model

Corresponding to the infective dose, probability methods are generally adopted to assess infection risk, which leads to the development of risk assessment models. Two types of model have been developed for the risk assessment of infection transmission, which are the Wells-Riley model and dose-response model, respectively.

2.8.1 Wells-Riley model

The Wells-Riley model is based on the Poisson probability distribution [165]. This model introduces a hypothetical infective dose unit, the quantum of infection, which is estimated by backward fitting the attack rate data of disease during an outbreak. The original model has been modified to consider more influencing factors of infection risk. For instance, Nazaroff et al. [166] add the disinfection effect of

ultraviolet irradiation and the filtration effect of filter into the model. The airborne persistence and deposition loss of pathogen are included by the model of [167]. As Sze To and Chao [168] comment, however, the persistence of pathogen and deposition loss have already been implicitly considered by the original model [165], during the backward calculation of the quanta generation rate. The modified models including more factors may lead to the repeated consideration of these factors for risk assessment. Since the effect of pathogen resuspension may have also been considered during the backward calculation of the quanta generation rate, it is inappropriate to consider the role of pathogen resuspension on infection transmission using the Wells-Riley model.

2.8.2 Dose response model

The infection probability after exposing to a certain amount of pathogens could also be estimated by the exponential or beta-Poisson dose response models [162, 169]. The exponential dose-response model is

$$P_i = 1 - e^{-r_i I} \quad (2.17)$$

where r_i is the fitting parameter accounting for the infectivity of pathogen and the pathogen-host interactions. I is the amount of pathogens human is exposed to. The beta-Poisson dose response model is

$$P_i = 1 - \left(1 + \frac{I}{\epsilon_i}\right)^{-\alpha_i} \quad (2.18)$$

where α_i and ϵ_i are the fitting parameters accounting for the infectivity of pathogen and the pathogen-host interactions. These two dose response models are suitable for different pathogens, respectively. For example, among the five category A BW agents (*B. anthracis*, *Y. pestis*, *F. tularensis*, *Variola major* and *Lassa*), the dose response

relationship of the first three agents is the exponential one, while the dose response relationship of the last two agents is beta-Poisson one [21].

In order to apply a dose response model, it is necessary to know the fitting parameter(s) (i.e., r_i or α_i and ϵ_i) which can be estimated based on infective dose data. For many pathogens, the human infective dose data are not available and interspecies extrapolation is needed to transfer the existing animal data to humans. The influencing factors (e.g., pathogen persistence, deposition loss of pathogen, and pathogen resuspension) of infection transmission could be explicitly considered by the dose response model, once their influences towards human exposure (I) could be modelled. Hence, the dose response model will be adopted in this work to study the effect of AIPR and WIPR on infection transmission.

2.9 Conclusions

The knowledge about the influence of pathogen resuspension towards infection transmission indoors is still limited due to the lacking of data about resuspension processes. Both AIPR and WIPR could affect occupants' exposure to pathogens indoors but are poorly understood. AIPR could play an important role in the potential bioterrorist attack based on ventilation systems. In order to assess the risk of bioterrorist attack through ventilation systems, a model that can predict BW agent concentration dynamics in the ventilation duct with AIPR is needed. In order to model WIPR, more experiments are needed. Once the models corresponding to AIPR and WIPR are developed, they can be substituted into the two-compartment mass balance models to model airborne and surface concentrations. The exposure analysis could be

conducted based on the modelled concentrations. A risk assessment scheme could then be developed by integrating the exposure analysis into the dose response model with the knowledge of biological information of pathogens. Further effort should also be put to improve the current capability of theoretically modelling AIPR. A turbulent bursts-based model considering (1) the adhesion force distribution, (2) the depletion of resuspendable particles and (3) the effect of RH will be desirable for such purpose. Correspondingly, the current understanding of particle-surface adhesion force needs to be improved. In the following chapters, studies will be conducted to fill the existing knowledge gaps about AIPR and WIPR and their impacts on infection transmission.

Chapter 3 Particle Concentration Dynamics in the Ventilation Duct with AIPR

3.1 Introduction

Terrorists could deliberately place BW agents onto the duct surface when the ventilation system is off (usually at night, therefore more covert). Some of these agents could be resuspended and transported into indoor environment once the ventilation system is turned on, leading to mass contamination [32-34]. In order to assess the risk due to this kind of bioterrorist attack, it is necessary to develop a model that can predict the BW agent concentration dynamics in the ventilation duct with AIPR.

Despite the importance of relevant knowledge about the concentration dynamics in the ventilation duct following a BW agent resuspension event, few studies have been conducted in this area. Until recently, Zhou et al. [14] propose a model for the particle concentration dynamics in the ventilation duct considering resuspension. However, their model is constructed based on the assumption that both the particle deposition and resuspension occur uniformly along the whole length of ventilation duct. This naturally makes their model inappropriate for cases where high concentration of particles are dosed in a small area in the duct and the initial resuspension occurs from that small area, usually in the case of a bioterrorist attack. The governing equation in [14] is specifically organized to have a term accounting for the particle resuspension along the whole length. In the case of resuspension from a small area, this governing equation in [14] no longer holds and a simple substitution of the resuspension term in

their governing equation is not physically reasonable. A different method is needed to solve the new governing equation corresponding to the case that initial resuspension occurs from a small area. Based on the mass balance approach, this chapter proposed a new model for particle concentration dynamics in the ventilation duct with AIPR in the case of a bioterrorist attack. The proposed model was validated by a series of wind tunnel experiments. The spatial variation of particle concentration in the duct after resuspension was also explored based on the proposed model.

3.2 Model derivation

The particles deposit (primary deposition) on a small area in the duct and are subsequently resuspended (primary resuspension) into the airflow stream when the ventilation is turned on. Only the initial (primary) resuspension is considered here, because (1) it plays the dominant role in affecting the airborne particle concentration over the secondary resuspension (subsequent resuspension of particles deposited on the duct surface downstream); (2) the amount of particles for secondary deposition is small and the amount for secondary resuspension would be even far smaller than that for secondary deposition, meaning that the net deposition could be well approximated by the secondary deposition; (3) further considering the secondary resuspension will be a traversal problem that is prohibitive to solve. The transient particle concentration variation along the streamwise direction, $C_{ov}(x, t)$ is concerned in the proposed model. Particle concentration is assumed homogenous in the cross-section at any given point in x and t . As shown in Figure 3.1, the particle resuspension occurs within the area of S_v (dose area of BW agents) where the particle surface number concentration is N_0 . The particle concentration upstream the resuspension area is C_0 , while the particle

concentration downstream the resuspension area is $C_{ov}(x, t)$. According to the conservation of mass, the mass balance equation about $C_{ov}(x, t)$ can be written as:

$$A_v \frac{\partial C_{ov}(x, t)}{\partial t} + Q_s \frac{\partial C_{ov}(x, t)}{\partial x} = -V_d C_{ov}(x, t) P_v \quad (3.1)$$

with the boundary condition of

$$C_{ov}(x, t)|_{x=0} = C_0 + \frac{N_0 S_v \Lambda(t)}{Q_s} \quad (3.2)$$

and the initial condition of

$$C_{ov}(x, t)|_{t=0} = C_{t0}, \quad (3.3)$$

where A_v is the cross-sectional area of duct, Q_s is the volumetric flow rate, V_d is the overall deposition velocity of particles in the duct, P_v is the cross-sectional perimeter of duct and Λ is the normalized resuspension rate. As reviewed in Chapter 2, the normalized resuspension rate generally has a power law relationship versus time: $\Lambda = r_{n1} t^{-r_{n2}}$ [98, 109, 116]. After plugging the resuspension rate expression into Eq. (3.1), the solution of Eq. (3.1) is derived as (See Appendix A):

$$C_{ov}(x, t) = \begin{cases} C_{t0} e^{-\frac{V_d P_v t}{A_v}} & (0 < t \leq \frac{A_v x}{Q_s}) \\ \frac{N_0 S_v r_{n1}}{Q_s (t - \frac{A_v x}{Q_s})^{r_{n2}}} e^{-\frac{V_d P_v x}{Q_s}} + C_0 e^{-\frac{V_d P_v x}{Q_s}} & (\frac{A_v x}{Q_s} < t) \end{cases} \quad (3.4)$$

In Eq. (3.4), $\frac{A_v x}{Q_s}$ defines the time when the location x will be affected by the resuspended particles. That is, when $0 < t \leq \frac{A_v x}{Q_s}$, the location x will have a concentration variation affected by the deposition only. Otherwise, the location x will have a concentration variation influenced by both particle resuspension and deposition.

Figure 3.1 A schematic diagram of the particle resuspension in a duct.

Considering that the particle deposition velocities onto the floor, wall and ceiling are different due to the effect of gravity, Eq. (3.4) is modified to

$$C_{ov}(x, t) = \begin{cases} C_{t0} e^{-\frac{(v_{dfv}P_{fv}+v_{dwv}P_{wv}+v_{dcv}P_{cv})t}{A_v}} & (0 < t \leq \frac{A_v x}{Q_s}) \\ \frac{N_0 S_v r_{n1}}{Q_s (t - \frac{A_v x}{Q_s})^{r_{n2}}} e^{-\frac{(v_{dfv}P_{fv}+v_{dwv}P_{wv}+v_{dcv}P_{cv})x}{Q_s}} + C_0 e^{-\frac{(v_{dfv}P_{fv}+v_{dwv}P_{wv}+v_{dcv}P_{cv})x}{Q_s}} & (\frac{A_v x}{Q_s} < t) \end{cases} \quad (3.5)$$

where v_{dfv} , v_{dwv} and v_{dcv} are the deposition velocities of particles onto the floor, wall and ceiling of duct respectively, and P_{fv} , P_{wv} and P_{cv} are the width of floor, wall and ceiling respectively. The estimation of deposition velocities onto different surfaces of duct will follow the reported method in [132]. The particle surface number concentration N_0 is calculated as

$$N_0 = \frac{M_{or} f_p}{S_v m_p}, \quad (3.6)$$

where M_{or} is the mass of particles released to the surface for resuspension. m_p is the mass of a particle. f_p denotes the fraction of deposited particles belonging to the size bin of d_p , which can be obtained from the particle size distribution. The normalized resuspension rate is estimated based on the previous empirical models of Loosmore [116] or Kim et al. [98]. Two models and three models have been developed in [116]

and [98], respectively. Because different models from the same study generally produced similar results, one model from each of these studies was used: emp1 (Eq. (2.11)) from [116] and Model II-A (Eq. (2.13)) from [98]. The particle concentration dynamics models based on emp1 (Eq. (2.11)) and Model II-A (Eq. (2.13)) are denoted as Model 1 and Model 2, respectively. RH will also affect AIPR by affecting the capillary force between particles and surfaces as will be shown by the development of adhesion force models in Chapter 7 and 8. In Chapter 9, a theoretical AIPR resuspension model will be proposed with the capability of predicting the effect of RH on AIPR. It should be noted that the model (Eq. (3.5)) of particle concentration dynamics in the duct with AIPR was developed based on the existing empirical resuspension models (Eq. (2.11)) and (Eq. (2.13)). These empirical models generally provide reasonable predictions against experimental data, without considering the parameter of RH. Once the empirical models are improved in the future with the consideration of RH, the developed airborne concentration model will be improved correspondingly.

3.3 Validation experiments

3.3.1 Surface roughness measurement

The surface roughness of substrate is required for estimating the normalized resuspension rate. Three types of material (stainless steel (SS), aluminum (AL) and plastic (PL)) were tested, as they are common materials for the construction of ventilation ducts [170-173]. 5 pieces of 4 cm $\times$ 4 cm square-shaped substrate were prepared from each material and the roughness of each substrate was measured using

a surface roughness tester (Mitutoyo, SJ301) at three random locations. The average RMS roughness for each material was calculated and listed in Table 3.1. The other parameters required for the resuspension rate calculation are also given in Table 3.1.

Table 3.1 Parameters required for the normalized resuspension rate estimation.

Substrate	u^* (m/s)	ρ_p (kg/m ³)	ρ_a (kg/m ³)	d_p (μ m)	σ_1 (μ m)	$A_h^{\ddagger}(\times 10^{-20}\text{J})$
AL	0.278	2650	1.2	2/4.75	0.44	15.7
SS	0.278	2650	1.2	2/4.75	0.09	2.7
PL	0.278	2650	1.2	2/4.75	0.02	7.3

$\ddagger$: $A_h = \sqrt{A_{11}A_{22}}$, with A_{11} as the Hamaker constant of substrate and $A_{22} = 6.8 \times 10^{-20}$ J as the Hamaker constant of particles [98]. The Hamaker constants for aluminum, stainless steel and plastic are 36.0×10^{-20} [174], 1.0×10^{-20} [175] and 7.8×10^{-20} J [176], respectively.

3.3.2 Sample preparation by deposition procedure

A deposition chamber was used to load the test particles (ISO 12103-1 A1 Arizona test dust, Powder Technology, Inc.) onto the substrates to mimic BW agent dose during ventilation off period. The loaded substrates would be used for the subsequent resuspension experiments in a wind tunnel. The deposition chamber was made of stainless steel and had the inner dimensions of 60 cm (W) $\times$ 60 cm (H) $\times$ 60 cm (L). Four mixing fans (Paps, Series 8000N), each providing 50 m³/h of airflow rate were installed inside the chamber to provide air mixing. There was a circular inlet port at the centre of the ceiling through which test particles were injected into the chamber by a syringe (BD 10 cc syringe, Luer-Lok). In the deposition experiments, it was found that the number of particles deposited onto the walls were much fewer than that deposited onto the floor, as will be explained below. In this case, the size distribution of particles deposited on the substrates was assumed to be similar to that of the injected test particles. The cumulative size distribution of particles in terms of volume

is shown by Figure 3.2. The size of test particles ranges from 1 to 10 μm which covers the size ranges of some common BW agents such as *B. anthracis* and *Botulinum toxin* [46].

Figure 3.2 The cumulative size distribution of test particles.

Before the deposition, each piece of substrate was cleaned with tissue paper dipped with ethanol and then weighed by an analytical balance (Radwag XA 110/X, readability: 0.01 mg). Each weight measurement was taken one and a half minutes after the substrate was placed on the balance to ensure sufficient time for stabilizing the reading. The weight obtained at this stage was recorded as M_{1r} . Immediately after the weight measurement, the substrate was put into the deposition chamber. After placing all substrates into the chamber, the door of the deposition chamber was closed. The mixing fans in the chamber were then switched on. After 5 minutes, 2 grams of test dust were injected into the chamber from the inlet port on the ceiling of the chamber with a syringe by pulling and pushing the syringe rod repeatedly at a rate of 20 times/minute. The mixing fans remained on for another 5 minutes after the particle injection. Since the airflow rate of each fan was 50 m^3/h , 77 chamber volumes of air

were circulated during the 5-min period, which ensures adequate air mixing in the chamber. The mixing fans were then turned off and the chamber was left intact for 4 hrs to allow particle deposition. Based on the gravitational settling velocity of 7.3×10^{-3} m/s for 1 μm particles, it took about 2.5 hrs for the particle to fall down from the ceiling to the floor of the chamber. Therefore, 4 hrs of settling time were used to ensure that most of the test particles were deposited. The substrates were then taken out and weighed again by using the analytical balance. The weight obtained at this stage was recorded as M_{2r} . The deposited mass of particles is calculated as $M_{0r} = M_{2r} - M_{1r}$ and its respective data for various cases are listed in Table 3.2.

Table 3.2 The deposited mass of particles and the upstream particle concentration

	M_{0r} (g)	C_0 (#/m ³)	
		2 μm	4.75 μm
AL	0.01161 (0.00357) [†]	201650 (50010)	5817 (2007)
SS	0.01290 (0.00475)	225252 (72351)	3306 (1691)
PL	0.01347 (0.00480)	200367 (20991)	4282 (1670)

[†]: The standard deviations are shown within brackets.

An additional experiment was conducted to compare the particle masses deposited onto the floor and walls. Two gravimetric filters (47 mm PTFE filter with mass of M_{f1}) were placed horizontally (upward-facing) to the floor and another two filters were placed vertically (sideward-facing) to the wall. The two filters were placed at the centre and corner of the floor (wall), respectively. Then, the deposition procedure described above was followed and the filters were re-weighed (M_{f2}). The particle mass deposited on each filter was calculated by ($M_{f2} - M_{f1}$) and the average deposited mass for the filter on the floor was compared to that on the wall. It was found that the

average deposited mass for the filters on the floor (0.01611 g) was about 2 orders of magnitude larger than that on the wall (0.00019 g). This indicated that there was little amount of particles deposited onto the walls as compared with that deposited onto the floor. Hence, it could be assumed that all of the dispensed particles were deposited on the floor of the chamber where the test substrates were placed for particle loading.

3.3.3 Particle resuspension experiments

Resuspension experiments were conducted in a suckdown wind tunnel setup (Figure 3.3) with a test section of 20 cm (W) $\times$ 20 cm (H) $\times$ 100 cm (L). A flow straightener was installed in front of the contraction part to smooth flow and the turbulators were paved behind the contraction part to induce a turbulent boundary layer. A 23.5 cm (L) $\times$ 20.0 cm (W) supportive plastic substrate base with a 4.0 cm (L) $\times$ 4.0 cm (W) trough for fitting the test substrate was fixed in the test section. The distance between the center of the trough and the inlet of the test section was 48.5 cm. The substrate base has a 10° wedge to allow smooth change of flow direction. The speed of fan (Kruger Engineering Pte Ltd, FSA200/CM), i.e., the free stream velocity, was controlled by a frequency inverter. An aerosol spectrometer (Grimm, model 1.109) was employed with the probe 15 cm downstream the substrate to measure the particle concentration at the sampling interval of 6 s. The height of probe from the floor of test section was 9 cm.

Figure 3.3 A schematic diagram of the wind tunnel setup.

Before the resuspension experiment, the relationship between the friction velocity (required for calculating the normalized resuspension rate) and free stream velocity was determined based on the boundary layer velocity profile measured with a set of hot wire anemometer (developed by The University of Newcastle). A height gauge (Mitutoyo, series 192) was used to control the vertical movement of the anemometer probe. A pitot-tube with an inclined manometer (Airflow Developments Ltd) was used to measure the free stream velocity and calibrate the hot wire anemometer. The diameter of the pitot-tube is 0.2 cm which is significantly smaller than the dimension of the test section (20 cm (W) × 20 cm (H)). Hence, it could be assumed that the presence of the pitot-tube will have minor effect to the flow characteristics. Before the measurement of boundary layer velocity profile, the pitot-tube with the manometer was used to calibrate the hotwire anemometer following the method of [177]. Then, the boundary layer velocity profile was measured by traversing the anemometer probe from the height of 0.1 mm to 0.27 mm at the increment of 0.01 mm for each of six free stream velocities: 1.85, 2.45, 3.07, 3.59, 4.19 and 5.20 m/s. For turbulent boundary layers, the velocity profile can be formulated with the Prandtl equation:

$$u = \frac{u^*}{\kappa} \ln \left(\frac{z_u}{z_{u0}} \right), \quad (3.7)$$

where κ is the von Kármán constant ($\kappa = 0.41$), z_u is the vertical distance from the surface and z_{u0} is the aerodynamic roughness length. It should be noted that the presence of particles on the surface will affect the roughness length (z_{u0}) in the velocity profile equation (Eq. (3.7)), as the surface characteristics will be modified by the presence of particles. Specifically, when a great number of particles are present on surface and being resuspended, z_{u0} will not be constant, but vary with the free stream velocity [141, 178]. In the experiment, however, a sparse layer of particles are used for resuspension, therefore the effect of particle on changing surface roughness is assumed to be minor. Furthermore, the prediction of the normalized resuspension rate models (i.e., Eq. (2.11) and Eq. (2.13)) is based on the friction velocity corresponding to the turbulent boundary layer in the absence of particles. Hence, the velocity profile of the turbulent boundary layer in the absence of particles (Eq. (3.7)) is used. In order to determine the friction velocity, the recorded velocity data would be fitted by the Prandtl equation. Similar to the method introduced by [178], the velocity profile is shown as $\ln(z)$ versus u (Figure 3.4 (a)) and the friction velocity corresponding to each free stream velocity could be found based on the slope of the fitted curve. Finally, a linear relationship between the friction velocity and free stream velocity was found as illustrated in Figure 3.4 (b), where $u^* = 0.0710U_\infty - 0.0056$ with the residual sum of square $R^2=0.988$.

Figure 3.4 (a) The boundary layer velocity profiles at various free stream velocities. (b) The relationship between the friction velocity and free stream velocity.

The free stream velocity of 4.0 m/s ($Re = 53000$) was used in the resuspension experiments, which fell into the range of common free stream velocities in the ventilation ducts (2 - 9 m/s and $Re \approx 20000 - 60000$) [31]. An annular aspiration inlet was employed for particle sampling. Under the free stream velocity of 4.0 m/s, it

is estimated that the inlet has the overall sampling efficiency larger than 95% for particles smaller than 10 μm in size, according to the existing theory [179]. This suggested that an approximately isokinetic sampling condition was achieved. At the beginning of each resuspension experiment, the background concentration, the average of which served as the upstream concentration C_0 (Table 3.2) for the model prediction, was measured for two minutes. The substrate was then mounted on the substrate base in the wind tunnel for the resuspension experiment and the particle concentration in the tunnel was measured for another 2 minutes. For each material, all 5 pieces of substrate were tested in the resuspension experiments and the measured concentrations of them were averaged for the model validation. The RH and temperature in the wind tunnel were measured to be $85\% \pm 2\%$ and $27^\circ\text{C} \pm 2^\circ\text{C}$, respectively, using a RH-temperature sensor (OMEGA, RH-USB).

3.4 Results and discussion

3.4.1 Model validation

The time limit, $\frac{A_v x}{Q_s}$, (Eq. (3.5)), is 0.0375 s, which is significantly smaller than the sampling interval of 6 s. Therefore, the concentration variation as $0 < t \leq \frac{A_v x}{Q_s}$, in Eq. (3.5), is not considered in the following validation. The concentration variations due to the resuspension for the particles larger than 6.5 μm are very small, therefore they are not considered in the validation for the statistical significance of analysis. The considered particles were divided into 2 size bins: 1 – 3, 3 – 6.5 μm , with the denoted mean diameters of 2 and 4.75 μm , respectively. The estimated normalized resuspension rate and deposition velocities of various cases are shown in Table 3.3.

The model validation is shown by Figure 3.5. Since the spectrometer measured the concentration with the interval of 6 s, the time axis starts from 6 s in Figure 3.5.

Table 3.3 The normalized resuspension rate and deposition velocities of various cases.

Parameters			Substrate					
			AL		SS		PL	
d_p (μm)			2	4.75	2	4.75	2	4.75
$\Lambda = r_{n1}t^{-r_{n2}}$	Model 1	r_{n1}	0.0008	0.0009	0.0013	0.0015	0.0022	0.0025
		r_{n2}	0.92	0.92	0.92	0.92	0.92	0.92
	Model 2	r_{n1}	0.0018	0.0053	0.0052	0.0151	0.0063	0.0183
		r_{n2}	1.0135	1.0135	1.0135	1.0135	1.0135	1.0135
	v_{dfv} (m/s)		0.0014	0.0058	0.0014	0.0058	0.0014	0.0058
	v_{dwv} (m/s)		0.0005	0.0018	0.0005	0.0018	0.0005	0.0018
v_{dcv} (m/s)		0.0010	0.0031	0.0010	0.0031	0.0010	0.0031	

It is shown that the concentration dynamics after the particle resuspension is reasonably captured by the proposed model. Both the experimental and modeling results show that the particle concentration becomes 1.5 – 3 times and 4 – 8 times higher than the upstream one immediately after the initiation of airflow for 2 μm and 4.75 μm particles, respectively, and gradually decreases afterwards. Once the airflow was initiated, the airflow resuspended the particles on the substrate and quickly pushed them forwards the measurement point, leading to the significant concentration increase. The subsequent concentration decline was mainly caused by three aspects based on the proposed model: (1) the normalized resuspension rate decreases as the time goes on; (2) the ventilation continuously refreshes the air in the tunnel (dilution effect); (3) some of the resuspended particles deposit onto the duct surfaces. Hence, there is a critical time when the particle concentration will become smaller than the

initial concentration (C_{t0}), as the effect of AIPR on airborne concentration is overtaken by that of ventilation and deposition. The influential factors (e.g., deposition velocity, size of ventilation duct and number of resuspendable particles) of the critical time are shown by the proposed airborne concentration model (Eq. (3.5)). A scaling law may be developed using Buckingham π theorem, but a lot more experiments are needed, which will be left as a future study.

Figure 3.5 The comparison between the measured and modeled concentration variations after particle resuspension for the substrates of (a) aluminum (i: 2 μm ; ii: 4.75 μm), (b) stainless steel (i: 2 μm ; ii: 4.75 μm) and (c) plastic (i: 2 μm ; ii: 4.75 μm). The error bars denote one standard deviation.

The comparison between the model predictions based on the empirical resuspension model of [116] (Model 1) and those based on the one of [98] (Model 2) shows that the latter-based model provides larger but generally better predictions than the former-based model. The larger predictions for the model based on Model 2 correspond to the calculated larger resuspension rate coefficients, r_{n1} (Table 3.3).

3.4.2 Spatial concentration variation after resuspension

The spatial concentration variation along the duct after resuspension at different points of time (10, 20, 30 s) is explored using the proposed model. The duct length is accounted by putting the dosing location at origin. The case of 2 μm particles on the plastic substrate experimentally examined above is used. All other parameters required by modeling are kept the same as above. The result is shown in Figure 3.6.

Figure 3.6 The spatial variation of particle concentration in the duct at various time points (10, 20 and 30 s) after resuspension.

It is shown by Figure 3.6 that the particle concentration increases along with the duct until the critical point (the concentration peak) which is the furthest location the airflow carrying resuspended particles could reach by the time. The particle concentration at the critical point decreases with time (10 – 30 s) because more particles are lost due to deposition for longer time. This decrease in concentration is about 16% of the peak concentration at the critical point, suggesting that the deposition has a minor impact on the concentration for 2 μm particles, compared to the primary resuspension. Further down from the critical point, the particle concentration is not affected by the primary resuspension but decreases slowly due to deposition, compared to the initial concentration, C_{i0} . The above conclusions also hold for the case of larger particles (e.g., 10 μm , not shown here to avoiding repetition).

3.5 Conclusions

Ventilation ducts serve as a potential vehicle for the dispersion of harmful agents in case of a bioterrorist attack. In this chapter, the model for predicting the particle concentration dynamics in the ventilation duct with AIPR was derived based on the mass balance equation and empirical AIPR models. A series of wind tunnel experiments were conducted for validating the proposed model. It was found that the particle concentration increased immediately after the initiation of airflow in the duct and gradually decreased as the time went on. The spatial particle concentration variation along the duct after resuspension was further explored using the proposed model. It was found that the concentration increased downstream until reaching a critical point after which the concentration dropped sharply to the background level. The proposed model could provide the foundation for predicting the BW agent concentration in the supply air and in the occupied space in the case of a related bioterrorist attack.

Chapter 4 Experimental Investigation and Modeling of WIPR

4.1 Introduction

Although some knowledge has been accumulated about WIPR, the effects of some factors such as walking rate, RH, and mechanisms on WIPR have been rarely explored. Studies on modelling the airborne concentration profile during human walking are also rare. Developing models for walking-induced resuspension is important to particle exposure estimation. This chapter intends to supplement the data bank for WIPR and derive an airborne particle concentration model with human walking involved. WIPR was investigated using controlled experiments conducted in a setup consisting of a deposition chamber and a resuspension chamber into which a pair of motorized model legs was installed. The resuspension rate was calculated based on a mass balance model and the power law was used to fit the resuspension rate data. The effects of flooring material, particle size, walking rate, and RH on WIPR were examined. The importance of the pure aerodynamic mechanism on resuspension was compared with the contact mechanism by controlling the floor touching of the feet in the experiments. Based on the fitted power law relations, the model of airborne particle concentration during the walking period was derived.

4.2 Methodology

4.2.1 Experimental setup

4.2.1.1 Deposition chamber

The experimental setup, as shown in Figure 4.1, consists of two main components: a deposition chamber and a resuspension chamber. The deposition chamber was used for the deposition procedure, in which test particles were loaded on flooring samples. The loaded flooring samples would be used for the subsequent resuspension experiment in the resuspension chamber. The detailed specifications of deposition chamber could be found in Chapter 3.

Figure 4.1 A schematic diagram of the experimental setup and procedure.

4.2.1.2 Resuspension chamber

The resuspension experiments were conducted in the resuspension chamber made of stainless steel with the inner dimensions of 60 cm (W) $\times$ 45 cm (H) $\times$ 80 cm (L). The front side of the chamber had a transparent acrylic panel for visual monitoring of the experimental process. This acrylic panel was removable to allow for loading and unloading the flooring samples. In each resuspension experiment, six flooring samples, 15.0 cm $\times$ 12.5 cm each, were placed beneath each foot in a 2-by-3 arrangement and

work like a large single piece. The flooring samples were pre-loaded with test particles by the deposition procedure. In this study, 3 types of flooring material were tested, including carpet, vinyl and wood PVC (PVC plate mimicking the appearance of wood). A pair of motorized model legs was installed inside the resuspension chamber. The feet attached to the motorized legs were made from acrylic plates with the shape and size of a men's size 8 shoe. During the experiments, the feet fell onto the same place of flooring samples beneath. The model legs performed stomping-like walking activity driven by a direct current motor mounted on the top of the chamber. The driving motor was powered by a variable direct current power supply (InStek GPS – 3030DD), where the walking rate was controlled and adjusted. A trial calibration was firstly conducted to determine the walking rate for experiments, in terms of steps per minute made by the feet. One step refers to the process of one foot moving up and down. Three walking rates, 84, 108, and 132 steps per minute, were chosen for the subsequent resuspension experiments. The adopted rates were similar to the optimum walking rate recommended by the study of Rowe et al. [180], where the walking rate of 90 – 113 steps per minute was recommended as moderate-intensity walking for adults to gain health benefits. The distance between the feet and the flooring samples had 2 settings in the walking motion. One setting was that the feet were in contact with the flooring samples when the feet were fully down. In this setting, both the airflow generated by feet movement and the physical contact contributed to resuspension (the **contact** case). The other setting left a 4 mm gap between the feet and the flooring samples when the feet were fully down, meaning that there was no physical contact between the feet and flooring samples in this setting, i.e., only the airflow generated by the foot movement contributed to the resuspension (the **aerodynamic** case). An aerosol spectrometer (GRIMM model 1.109) was fitted

to monitor the mass concentration of PM_{10} and $PM_{2.5}$ (particulate matters of sizes $\leq 2.5 \mu m$) inside the resuspension chamber in real-time at 6-second intervals. The sampling inlet of the aerosol spectrometer was placed at 9 cm from the left-side wall and 10 cm from the floor of the chamber. The RH and temperature in the chamber were monitored with an RH-temperature sensor (OMEGA, RH-USB) mounted on the right-side wall. The temperature inside the chamber was 28.0 ± 2.1 °C during the experiments.

4.2.2 Experimental procedure

4.2.2.1 Flooring samples preparation – deposition procedure

Before each resuspension experiment, a deposition procedure similar to the one described in Chapter 3 was carried out to load the test particles onto the flooring samples. For each experiment, 12 flooring samples (6 for each foot) were prepared through the deposition procedure. The weights of each flooring sample before and after the deposition procedure were denoted as M_1 and M_2 , respectively. Based on the weight differences ($M_2 - M_1$) of 12 material pieces in each experimental run, an uniformity index defined as the exponential of the negative CV (coefficient of variation) was calculated according to [181]. The index ranges from 0 to 1 and a value of 1 means that there is perfect uniformity. The calculated uniformity index was 0.61 ± 0.086 for all deposition experiments. Thus, reasonable uniformity was achieved in this study.

4.2.2.2 Resuspension experiment

Before each resuspension experiment, the interior of the resuspension chamber and the model feet were vacuum-cleaned. The flooring samples prepared by the deposition procedure were then placed into the resuspension chamber immediately after weighing for M_2 . The chamber was closed by bolting down the acrylic cover panel. Then, the aerosol spectrometer started sampling at 6-second intervals. Each resuspension experiment consisted of 3 stages and lasted for 20 minutes in total. In Stage 1, the leg movement mechanism remained off and the background particle concentration was monitored for 5 minutes. Then (Stage 2), the power supply to the leg mechanism motor was set to the desired voltage and switched on to actuate the walking motion for 5 minutes. The power supply to the leg motor was then switched off while the aerosol sampling continued for another 10 minutes to monitor the post-event PM concentration (Stage 3). After finishing the 3 stages, the flooring samples were removed from the chamber, vacuum-cleaned, and stored for the next experiment. It should be noted that this work used the stomping-like walking with a pair of motorized model legs to represent idealized human walking. The stomping-like motion was used in a number of previous studies and was found to be able to characterize the fundamental aerodynamics (jet and vortex motion) during walking pertinent to particle resuspension [122, 182, 183]. The aerodynamic mechanisms of resuspending particles are similar between the stomping-like walking and the walking with foot rotation. It was shown that both particle resuspension and particle redistribution occurred during the upward and downward motions for both the stomping-like walking and the walking with foot rotation [184], which suggested the similarity between these two walking styles in term of the particle resuspension.

4.2.3 Parameters

Three common indoor flooring materials— carpet, vinyl, and wood PVC — were tested in this study to investigate the impact of flooring material on WIPR. These materials were newly bought and pre-vacuumed before each experiment. In order to examine the effect of particle size, the aerosol spectrometer took readings of $PM_{2.5}$ and PM_{10} , respectively.

Some previous studies [15, 16, 18] have mentioned that WIPR can be influenced by the vigorousness of walking which is related to the walking rate. Therefore, the experiments were conducted under various controlled rates to understand the relationship between WIPR and the walking rate. Three walking rates — 84, 108, and 132 steps/min — were used in the experiments to study the effect of the walking rate.

The effect of RH on WIPR is another aspect that has been rarely studied. RH could influence the particle-surface capillary force and, thus, the particle resuspension from the surface as will be shown in Chapter 7 and 9. In order to adjust the humidity in the resuspension chamber, packages of desiccant (Water Jumbo, FairPrice) were placed at the corners of the chamber after the flooring samples have been put into the chamber. Then, the chamber was closed and dehumidified for 16 hrs. For the control group, no desiccant was used but the chamber was left alone for 16 hrs as well. The RH achieved by using five and two packages of desiccant and without using desiccant was 41%, 63% and 82% respectively. Carpet and vinyl were used to test the humidity effect. Except for the experiments examining the humidity effect, all other resuspension experiments were performed immediately after the resuspension chamber was closed.

Particle resuspension could be caused by either the aerodynamic mechanism or mechanical mechanism or both, as introduced by the previous studies [185, 186]. Gomes et al. [22] examined the effect of airflow and vibration towards resuspension with the experiments in a scaled chamber. The aerodynamic mechanism refers to the actions of air turbulence, such as sweeping eddies and viscous shear forces. The mechanical mechanism refers to the actions of mechanical disturbance such as vibration and contact. Both the aerodynamic mechanism and mechanical mechanism contribute to WIPR. Investigating these mechanisms separately will be meaningful for understanding their individual roles in the resuspension. The experiments investigating the aerodynamic mechanism of particle resuspension were conducted by adjusting the down position of the model feet to 4 mm above the flooring samples so that the acrylic feet would not touch the flooring in the down position. Except for the experiments testing the aerodynamic mechanism, all other experiments were conducted with the feet touching the floor.

4.3 Data analysis

4.3.1 Resuspension rate calculation

Figure 4.2 The sixth order polynomial fitting of the particle concentration variation during Stage 2 for wood PVC under the walking rate of 132 steps/min (contact case).

The sixth order polynomial function was used to smooth the concentration profile of Stage 2 for the following resuspension rate calculation (Figure 4.2). The reasons of using a sixth-order polynomial are that: (1) it helps to smooth the experimental data, which facilitates the numerical analysis of mass balance model; (2) it could fit the experimental data well with the R-squared value larger than 0.96, which ensures the accuracy of numerical analysis. For the time being, it is still difficult to assign a physical basis for this selection. Sources and sinks associated with the airborne particle concentration inside the resuspension chamber include the resuspension, deposition, sampling flow rate of the spectrometer, and inflow from outside of chamber to compensate the air extracted by the spectrometer. The coagulation of particles is neglected because it is relevant to ultrafine particles ($< 0.1 \mu\text{m}$) at high particle concentrations [187]. The resuspension rate, $R(t)$, defined as the amount of

particles resuspended per unit time, can be calculated based on the mass balance model, Eq. (4.1).

$$V_c \frac{dC_c}{dt} = R - \beta_p V_c C_c - \dot{V}(C_c - C_{oc}), \quad (4.1)$$

where $V_c = 0.216 \text{ m}^3$ is the volume of the chamber, $C_c (\mu\text{g}/\text{m}^3)$ is the PM concentration in the chamber, C_{oc} is the PM concentration outside the chamber, $\dot{V} = 2.0 \times 10^{-5} \text{ m}^3/\text{s}$ is the sampling rate of the aerosol spectrometer, $\beta_p (1/\text{s})$ is the particle decay rate loss coefficient due to particle deposition and $R (\mu\text{g}/\text{s})$ is the resuspension rate. The decay rate loss coefficient β_p has the order of magnitude of 10^{-3} s^{-1} . Since the loss due to air sampling (the 3rd term on the right hand side of Eq. (4.1)) was about 2 orders of magnitude smaller than the deposition loss (the 2nd term on the right hand side of Eq. (4.1)), it is neglected in the following analysis. Rearranging Eq. (4.1) yields

$$R(t) = V_c \frac{dC_c}{dt} + \beta_p V_c C_c. \quad (4.2)$$

Applying a forward difference approximation to $\frac{dC_c}{dt}$ in Eq. (4.2), the resuspension rate, $R(t)$ at the time $(t + \Delta t_s)$ can be obtained by

$$R(t + \Delta t_s) = V_c \frac{C_c(t + \Delta t_s) - C_c(t)}{\Delta t_s} + \beta_p V_c C_c(t), \quad (4.3)$$

where the time step $\Delta t_s = 6 \text{ s}$ was the sampling interval of the aerosol spectrometer. The estimation of β_p was based on the post-event PM concentration data (Stage 3) subtracted by the lowest mass in the experimental run. During this period of time, resuspension did not occur while deposition served as the sink of PM concentration in the chamber. Hence, Eq. (4.2) becomes

$$V_c \frac{dC_c}{dt} = -\beta_p V_c C_c. \quad (4.4)$$

Integrating Eq. (4.4) from 0 to t gives

$$C_c(t) = C_c(0)e^{-\beta_p t}, \quad (4.5)$$

where $C_c(0)$ is the PM concentration at the beginning of Stage 3. The exponential function was fitted to the concentration data for estimating β_p .

The calculated resuspension rate generally declined with time due to the depletion of resuspendable particles on the flooring samples and can be fitted by the power law as

$$R(t) = a_r t^{-b_r} . \quad (4.6)$$

The values of a_r and b_r for various cases are listed in Table 4.1. The resuspension rate, $R(t)$ depends on the surface particle concentration and particle resuspension area. Hence, $R(t)$ is divided by the initial surface particle concentration, $M(0)$, and resuspension area, S_r , to give the normalized resuspension rate:

$$\Lambda(t) = R(t)/[M(0)S_r]. \quad (4.7)$$

$\Lambda(t)$ will be used for investigating the influences of environmental conditions towards WIPR in the following part. $M(0)$ was calculated by

$$M(0) = \frac{\sum_{i=1}^{12} M_{2i} - \sum_{i=1}^{12} M_{1i}}{S_f}, \quad (4.8)$$

where M_{1i} and M_{2i} are, respectively, the weights of flooring sample i before and after the deposition procedure. $S_f=0.225 \text{ m}^2$ is the total area of 12 flooring samples. For PM_{10} , M_{1i} and M_{2i} are the measured weights, while for $\text{PM}_{2.5}$, they are calculated based on the size distribution shown by Figure 3.2 in Chapter 3. The data of $M(0)$ for various cases are listed in Table 4.1. The particle resuspension area is not just the area of modelled shoe sole, because the created wall jets (vortex structures) between the foot and floor could resuspend the particles on the flooring surface away from the sole. The existing measurements [182, 184] showed that the area about 6 cm away from the sole that was mimicked by a circular disk may be affected by the modelled walking

motion. The particle visualization experiment by Kubota et al. [184] showed that the particle resuspension area beneath one shoe spread away from the sole and was like a square shape for real walking motion. Hence, the particle resuspension area beneath the pair of shoes is approximated by $(0.26+0.06)^2 \times 2 = 0.2 \text{ m}^2$ for the men's size 8 shoes adopted by the experiment.

Table 4.1 Information about power law fittings and initial surface particle concentrations.

Flooring material	Relative humidity	Contact/Aero dynamic	Particle size	Walking rate	a_r	b_r	R-square	$M(0)/\text{gm}^{-2}$
Carpet	82%	Contact	PM ₁₀	132 steps/min	1.05	0.46	0.52	1.25
Carpet	82%	Contact	PM _{2.5}	132 steps/min	0.093	0.52	0.54	0.22
Carpet	82%	Contact	PM ₁₀	108 steps/min	0.96	0.49	0.60	2.75
Carpet	82%	Contact	PM ₁₀	84 steps/min	0.81	0.69	0.89	2.30
Wood	82%	Contact	PM ₁₀	132 steps/min	0.68	0.42	0.74	2.26
Wood	82%	Contact	PM _{2.5}	132 steps/min	0.16	0.68	0.74	0.40
Vinyl	82%	Contact	PM ₁₀	132 steps/min	0.93	0.62	0.91	2.46
Vinyl	82%	Contact	PM ₁₀	108 steps/min	0.58	0.71	0.81	2.09
Vinyl	82%	Contact	PM ₁₀	84 steps/min	0.29	0.79	0.66	4.06
Carpet	82%	Aerodynamic	PM ₁₀	132 steps/min	0.42	0.57	0.57	2.26
Wood	82%	Aerodynamic	PM ₁₀	132 steps/min	0.56	0.76	0.86	1.84
Carpet/RH	41%	Contact	PM ₁₀	132 steps/min	6.87	0.68	0.80	1.0
Carpet/RH	63%	Contact	PM ₁₀	132 steps/min	6.14	0.77	0.86	1.85
Carpet/RH	82%	Contact	PM ₁₀	132 steps/min	2.25	0.58	0.83	1.75
Vinyl/RH	41%	Contact	PM ₁₀	132 steps/min	3.22	0.51	0.62	3.18
Vinyl /RH	63%	Contact	PM ₁₀	132 steps/min	5.19	0.72	0.86	4.33
Vinyl /RH	82%	Contact	PM ₁₀	132 steps/min	2.27	0.61	0.81	4.33

4.3.2 Airborne particle concentration model involved with walking

Plugging the power law function of resuspension rate into the mass balance model, Eq.

(4.2), yields

$$V_c \frac{dC_c}{dt} + \beta_p V_c C_c = a_r t^{-b_r}, \quad (4.9)$$

which can be transformed to

$$\frac{d}{dt}(e^{\beta_p t} C_c) = \frac{a_r}{V_c} t^{-b_r} e^{\beta_p t}. \quad (4.10)$$

Integrating both sides of Eq. (4.10) from 0 to t and rearranging the equation give

$$C_c(t) = e^{-\beta_p t} C_c(0) + \frac{a_r}{V_c} e^{-\beta_p t} \int_0^t \frac{e^{\beta_p t}}{t^{b_r}} dt \quad (4.11)$$

which is the airborne particle concentration model involved with walking. The integration in Eq. (4.11) could be expressed in the form of incomplete gamma function, Γ_i , as

$$\begin{aligned} \int_0^t \frac{e^{\beta_p t}}{t^{b_r}} dt = \\ \{(-\beta_p)^{b_r-1} \Gamma_i[(1-b_r), 0] - t^{1-b_r} (-\beta_p t)^{b_r-1} \Gamma_i[(1-b_r), -\beta_p t]\}, \end{aligned} \quad (4.12)$$

The airborne particle concentration model (Eq. (4.11)) can be extended to a real indoor environment with β_p replaced by the sink of airborne particle concentration in the real case. The method applied for deriving the model (Eq. (4.11)) provides the basis for the development of more comprehensive airborne and surface pathogen concentration models in the following chapter.

4.4 Results and discussion

4.4.1 Investigations of factors and mechanisms affecting WIPR

The normalized resuspension rate ($\Lambda(t)$) is employed for investigating the influences of various factors and mechanisms towards WIPR.

4.4.1.1 Influence of particle size

The normalized resuspension rates of PM₁₀ and PM_{2.5} for different materials under the highest walking rate (132 steps/min) are shown by Figure 4.3. For the illustration purpose, the raw resuspension data of vinyl/PM₁₀ before fitting is also shown in the figure. Because the resuspension is not significant for the case of vinyl/PM_{2.5}, the resuspension rate of this case is not shown here. It is shown that the normalized resuspension rate of PM₁₀ is about 2.5 times that of PM_{2.5} for both carpet and wood PVC. The more significant resuspension for PM₁₀ should be related to the fact that the ratio between the detachment force and the adhesion force is smaller for smaller particles under the same condition as explained in [78, 90].

Figure 4.3 The comparison of the normalized resuspension rates of PM₁₀ and PM_{2.5} between different materials at the walking rate of 132 steps/min (contact case).

4.4.1.2 Influence of flooring materials

The comparison of the normalized resuspension rates of PM₁₀ from different flooring

materials is also shown by Figure 4.3. It is found that the normalized resuspension rate from carpet is about 2 and 4 times greater than those from wood PVC and vinyl, respectively. This might be caused by the difference of surface properties among different flooring materials. The surface of carpet is a layer of fibrous structure consisting of twisted tufts, whereas the surfaces of wood PVC and vinyl are relatively rigid and smooth. Therefore, unlike wood PVC and vinyl, the resuspension from carpet can be promoted by the vibration of the twisted tufts due to airflow or mechanical impingement of feet or both. Note that the normalized resuspension rate of $PM_{2.5}$ is also higher for carpet than for wood PVC in Figure 4.3.

4.4.1.3 Influence of walking rate

The comparison of the normalized resuspension rates between different walking rates (contact case) for carpet and vinyl flooring samples is shown by Figure 4.4. The lowest walking rate, 84 steps/min, represents slow and gentle walking indoors, while the highest walking rate, 132 steps/min, represents fast and vigorous walking indoors [188]. For carpet, the normalized resuspension rate at the highest walking rate is about 2.5 times of that at the medium walking rate and 7 times of that at the lowest rate. Whereas for vinyl, the normalized resuspension rate at the highest walking rate is about 2 times of that at the medium walking rate, and 10 times of that at the lowest rate. It is shown that the reduction of resuspension rate due to the lower walking rates for carpet is less significant than that for vinyl. This might suggest that the vibration of tufts is not significantly reduced in the lower walking rate cases, which makes the resuspension from carpet less dependent on the walking rate. The decreasing walking

rate results in a reduced normalized resuspension rate, because a lower walking rate induces smaller detachment forces.

Figure 4.4 The comparisons of the normalized resuspension rates of PM₁₀ between different walking rates for (a) carpet and (b) vinyl (contact case).

4.4.1.4 Influence of RH

The effect of RH on WIPR is shown by Figure 4.5. For both carpet and vinyl, the normalized resuspension rates under the low RH (41%) are, respectively, about 3 and 3.5 times of those under the medium (63%) and high (82%) RH. It is apparent that the change of normalized resuspension rate is more significant between the low and medium RH than between the medium and high RH. A likely cause of such difference is that the disappearance of menisci between the particles and flooring material due to humidity drop is much more significant between the medium and low RH than between the high and medium RH. This means that a greater reduction of the overall capillary force will be resultant when the RH decreases from medium to low level, which will also be found in Chapter 7. This result is consistent with the study by Thio [189], who found that the capillary force did not play a very significant role in dry pollen adhesion to carpet under 20% – 40% RH and the capillary force began to play a role when the RH was greater than 60%. The adhesion force between the particle and flooring material could be reduced due to the reduction of the capillary force for the low RH cases in this study, which leads to more particle resuspension.

Figure 4.5 The comparisons of the normalized resuspension rates of PM₁₀ between different RHs for (a) carpet and (b) vinyl (contact case) at the walking rate of 132 steps/min.

4.4.1.5 Influence of resuspension mechanism

The results presented above are all from the experiments with the model feet touching the floor (the contact case). To explore the aerodynamic effect on WIPR, the experiments were conducted for carpet and wood PVC with the feet not touching the

floor at the highest walking rate (132 steps/min). The aerodynamic case was similar to the fluid mechanics study by Kubota et al. [123], who investigated the particle resuspension in terms of the walking-induced flow field. Their findings indicated that particles were resuspended by a high velocity jet formed between the wall and the feet and that large-scale ring vortex structures pushed the resuspended particles away from the wall. In the current study, it was observed that some particles just beneath the edges of the feet were spread outward due to walking in a similar mode as that observed by Kubota et al. [123]. The comparison of the normalized resuspension rates of PM_{10} between the contact case and aerodynamic case is shown by Figure 4.6.

It is shown in Figure 4.6 that carpet has a higher normalized resuspension rate than wood PVC for both the contact and aerodynamic cases. It suggests that PM_{10} was more easily resuspended from carpet by both the aerodynamic and contact mechanisms than from wood PVC. In the wind tunnel experiments, Mukai et al. [190] also found that the resuspension for carpet is more significant than the relatively rigid and smooth materials such as linoleum and galvanized sheet metal. By using optical microscope, they found that most seeded particles were not imbedded deep into the carpet fibres but, instead, were located closer to the canopy surface. This deposit mode combined with the uneven lengths of carpet fibres made particles exposed to a higher velocity than particles on the smoother materials, which may lead to the more significant resuspension from carpet.

The normalized resuspension rates of the aerodynamic cases are about one eighth and one fifth of those of the contact cases for carpet and wood PVC, respectively. This indicates that including the mechanical mechanism is critical for WIPR and that the

particle resuspension could be considerably enhanced by combining this mechanism with the aerodynamic mechanism.

Figure 4.6 The comparison of the normalized resuspension rates of PM_{10} between the contact case and aerodynamic case for carpet and wood PVC at the walking rate of 132 steps/min.

4.4.2 Airborne particle concentration modelling

Previous researches [98, 109, 116, 191] have shown that the particle resuspension by unidirectional airflow has a power law relationship with respect to time (e.g., Eq. (2.11) and Eq. (2.13)). For WIPR where both the aerodynamic and mechanical disturbances exist, the power law relationship was also found to be able to fit the temporal variation of resuspension rate in this work. Based on Table 4.1, it could be found that the power exponent, b_r , ranged from 0.42 to 0.79 with the mean and standard deviation of 0.62 and 0.11, respectively and the power law coefficient, a_r , ranged from 0.093 to 6.83 with the mean and standard deviation of 1.91 and 2.17, respectively, for WIPR. The decay of resuspension rate for WIPR as time is due to the

fact that the relatively lightly adhered particles are resuspended leaving those tightly adhered particles, that is, the depletion of resuspendable particles.

In order to validate the airborne particle concentration model (Eq. (4.11)), the model predictions are compared with the experimental data of PM_{10} for carpet and vinyl at the highest walking rate (132 steps/min) and RH (82%). The comparison between the modelled PM_{10} concentration profiles and measured ones is shown in Figure 4.7. The modelled concentration profiles during human walking are in good agreement with measured ones: the modelled concentrations during walking based on Eq. (4.11) could capture the variation characteristic of experimental data. This means that the proposed power law relationship of resuspension rate versus time during walking is reasonable. It is possible to model the airborne particle concentration profile involved with human walking from Eq. (4.11), if the relevant parameters (e.g., R , V_c and β_p) are known. This might be of significance for the risk assessment of human exposure to harmful particles indoors with the occurrence of WIPR.

Figure 4.7 The comparison between the measured PM_{10} concentration profiles and modeled ones for different flooring materials at the highest walking rate (contact case).

Further model validation is conducted by comparing the model prediction with existing experimental data of Qian et al. [119]. In the study [119], the outdoor PM₁₀ concentration could be regarded to have minor influence to the indoor concentration and no other emission sources except resuspension existed. Hence, the major source for airborne particle concentration was the WIPR from the carpet flooring. The volume of indoor space, V_c , was 222 m³. The particle loss coefficient, β_p , was estimated to be 1 hr⁻¹ based on the concentration data without the resuspension, which is a reasonable value for a real indoor environment [5]. Since a normal walking was performed on the carpet flooring in the study [119], the resuspension rate ($R(t)=0.96\times t^{-0.49}$) of carpet/PM₁₀ at the medium walking rate serves as the reference case for determining the resuspension rate in the study [119]. The surface mass concentration of PM₁₀, RH and particle resuspension area were 1.2 g/m², 53% and 25 m², respectively, in the study [119], while they are 2.75 g/m², 82% and 0.2 m², respectively, in the reference case. Considering that the normalized resuspension rates for the RH cases of 41% and 63% were 3.5 and 3 times of that for the RH case of 82% as shown in Section 4.4.1.4, it is assumed that the normalized resuspension rate for the RH of 53% was 3.25 times of that for the RH of 82%. Therefore, the power law coefficient, a_r , of the resuspension rate for the study of Qian et al. [119] is estimated to be $[0.96\times(1.2/2.75)\times3.25\times(25/0.2)=170]$ according to the principle that the normalized resuspension rate of different cases should be proportional to each other. Therefore, the corresponding resuspension rate in the study of Qian et al. [119] is $R(t) = 170t^{-0.49}$, which would be employed for model predictions (Eq. (4.11)). The power law coefficient, a_r , is varied by 20% (i.e., $(1 \pm 20\%)a_r$) to account for the

effect of its uncertainty on the model prediction. The comparison between the model predictions and experimental data is shown in Figure 4.8. It could be seen that the model predictions well cover the measured airborne particle concentration variation during the walking. The observed increasing pattern of airborne concentration during walking is reasonably captured by the model predictions. This validates that the developed model (Eq. (4.11)) is effective to capture the airborne concentration variation due to WIPR.

Figure 4.8 The comparison of PM_{10} airborne concentration during the walking between the experimental data of Qian et al. [119] and model predictions.

4.5 Conclusions

The dependence of WIPR on particle size, flooring material, walking rate and RH was investigated experimentally in a chamber setup with a pair of model feet. The

resuspension mechanisms of human-walking were examined by comparing the experiments with and without the feet touching the floor.

The resuspension rate during the simulated walking activities was calculated based on the mass balance model and the power law was applied to fit the resuspension rate data. The resuspension rate was further normalized for investigating the effects of various factors on WIPR. It was found that the normalized resuspension rate of PM_{10} was about 2.5 times that of $PM_{2.5}$ for both carpet and wood PVC. Carpet had the highest resuspension rate, followed by wood PVC and vinyl. The reduction of normalized resuspension rate due to the lower walking rates was less significant for carpet than for vinyl. The normalized resuspension rate under low RH (42%) was significantly higher than the rates under the higher RH (63% and 82%). The normalized resuspension rate is much smaller in the aerodynamic case than in the contact case, indicating the critical role of mechanical mechanism for WIPR.

The time-dependence of the resuspension rate was found to follow the power law (Eq. (4.6)). The power exponent b_r ranged from 0.42 to 0.79 with the mean and standard deviation of 0.62 and 0.11, respectively, and the power law coefficient a_r ranged from 0.093 to 6.83 with the mean and standard deviation of 1.91 and 2.17, respectively, for the simulated walking. Based on the power law relationship, an airborne particle concentration model was developed. The developed model could predict the overall variation of airborne particle concentration involved with human walking. The method adopted to derive the model of this chapter also provides a hint for developing airborne and surface particle concentration models in the following chapter.

Chapter 5 Indoor Particle Concentration Models

Considering Particle Resuspension Processes

5.1 Introduction

The airborne and surface particle concentration models considering potential resuspension processes related to indoor environments were developed based on the two-compartment (air and surface compartment) mass balance models, Eq. (2.14) and Eq. (2.15) in Chapter 2. The considered resuspension processes included AIPR in the ventilation duct (Chapter 3) and WIPR indoors (Chapter 4). Outdoor sources and other potential indoor emission sources were included in the mass balance models. The particles outdoors could be transported indoors via mechanical or natural ventilation. Other indoor emission sources relevant to infection transmission might include expiratory activities and aerosolization of harmful pathogens indoors during a bioterrorist attack, etc.

In this chapter, the emission dynamics of various sources was firstly identified and mathematically modelled. The emission dynamics models were then substituted into the two-compartment mass balance models to develop a set of analytical airborne and surface particle concentration models. The derived models were validated against existing experimental data.

5.2 Model development

In order to model the variation of indoor particle concentrations, the emission dynamics of outdoor and indoor sources needs to be identified. The outdoor concentration C_o is applied in the mass balance model for representing outdoor sources. The indoor sources considered here are walking, dancing and vacuum cleaning, expiratory activities and aerosolization of harmful pathogens indoors such as that during a bioterrorist attack.

5.2.1 Emission dynamics

5.2.1.1 Outdoor source

If there is sudden mass emission(s) outdoors such as that from a large-scale bioterrorist attack, the outdoor airborne concentration could rise quickly during the period of mass emission. In this case, the variation of outdoor concentration could be approximated by the sum of two exponentials, $C_o = B_1 e^{-B_3 t} + B_2 e^{-B_4 t}$ as suggested by the previous urban air quality model [192]. When the mass emission ceases, the outdoor concentration will decay exponentially as time until to the background level due to various loss mechanisms such as deposition and wind-induced dilution [193]. The exponential decay, in this case, is actually a special case of the sum of two exponentials (either B_1 or B_2 is zero). Without sudden mass emission, the outdoor particle concentration will generally fluctuate around a mean value on both a yearly and daily basis [194-198]. Fully accounting for this fluctuation is impossible at the moment, because too many complicated and even undetermined factors such as meteorological conditions and location exist. The outdoor concentration is approximated by a constant value, that is, $C_o = A$, in this case. The constant outdoor concentration is also a special case of the sum of two exponentials, because the sum

of two exponentials devolves to the constant form with $A = B_1 + B_2$, when B_3 and B_4 are equal to zero. Hence, the sum of two exponentials is used for representing the potential variation of outdoor particle concentration.

5.2.1.2 AIPR in the ventilation duct

As described in Chapter 3, when BW pathogens are dosed onto ventilation duct surface when the ventilation is off, these pathogens will be resuspended (AIPR) and transported indoors when the ventilation is running again. This AIPR case is considered in the mass balance models by employing the particle concentration dynamics model developed in Chapter 3 (Eq. (3.5)). In Eq. (3.5), the effect of particle deposition in the duct was taken into consideration. Since the effect of particle deposition in the duct has already been considered by a_2 in the air compartment mass balance model (Eq. (2.14)), Eq. (3.5) needs to be modified to avoid repetition. The particle concentration in the duct resultant from AIPR without considering the particle deposition in the duct is

$$C_{ov}(t) = \frac{N_0 S_v r_{n1}}{Q_s t^{r_{n2}}} \quad (5.1)$$

where N_0 is the total number of pathogens dosed, Q_s is the ventilation rate in the duct. r_{n1} and r_{n2} are the power coefficient and exponent of the normalized resuspension rate for AIPR.

5.2.1.3 WIPR

As shown in Chapter 4, the resuspension rate, $R(t)$, could be applied in the mass balance models to account for the effect of WIPR. It was found that the variation of

resuspension rate with respect to time for WIPR could be described by a power law function. Considering the similarity among the activities of walking, dancing and vacuum cleaning, the emission dynamics of all these activities are described by the power-law resuspension rate: $R(t) = a_r t^{-b_r}$. a_r depends on the factors such as walking strength, particle surface loading, RH, resuspension area and flooring material, while b_r was found in the range from 0.42 to 0.79 [15, 199].

5.2.1.4 Other indoor sources

The emission is controlled by the particle producing process for the indoor sources such as expiratory activities and aerosolization of harmful pathogens indoors during a bioterrorist attack. The emission rate, E , (the number or mass of particles emitted per unit time) of these sources is assumed to be constant (i.e., $E = D$) during the period of emission, as adopted by existing studies [162, 166, 200]. The summary about the emission dynamics of the considered outdoor and indoor sources is shown in Table 5.1.

Table 5.1 Emission dynamics of various sources.

Source		Parameter	Unit	Mathematical model
Outdoor	With or without sudden mass emission	Concentration	#/ m^3	$C_o(t) = B_1 e^{-B_3 t} + B_2 e^{-B_4 t}$
	accident			
Ventilation duct	AIPR	Concentration	#/ m^3	$C_{ov}(t) = \frac{N_0 S_v r_{n1}}{Q_s t^{r_{n2}}}$
	WIPR	Resuspension rate	#/s	$R(t) = a_r t^{-b_r}$
Indoor	Expiratory activities and aerosolization of harmful pathogens	Emission rate	#/s	$E = D$

5.2.2 Model derivation

The two-compartment mass balance models (Eq. (2.14) and Eq. (2.15) in Chapter 2) are employed to derive the airborne and surface concentration models. The mass balance models are under the assumption of well-mixed (i.e., the airborne and surface concentrations are uniform), which has been widely adopted for modeling indoor particle concentration variation [15, 126, 137, 201]. It is assumed that the effects of nucleation, condensation and coagulation are negligible and the particle deposit structure has minor effect on resuspension rate estimation. It is also assumed that the emission rates of other indoor sources (E) are constant. Substituting $C_o(t) = B_1 e^{-B_3 t} + B_2 e^{-B_4 t}$, $C_{ov}(t) = \frac{N_0 S_v r_{n1}}{Q_s t^{r_{n2}}}$, $R(t) = a_r t^{-b_r}$ and $E = D$ from Table 5.1 into Eq. (2.14) yields

$$\begin{aligned} \frac{dC_i}{dt} = & a_1 (B_1 e^{-B_3 t} + B_2 e^{-B_4 t}) + a_2 \left(\frac{N_0 S_v r_{n1}}{Q_s t^{r_{n2}}} \right) - b C_i \\ & + \frac{a_r}{V t^{b_r}} + \frac{D}{V}. \end{aligned} \quad (5.2)$$

Substituting $R(t) = a_r t^{-b_r}$ into Eq. (2.15) yields

$$\frac{dM}{dt} = C_i v_{df} - \frac{a_r}{S_r t^{b_r}}. \quad (5.3)$$

Let $\frac{a_2 N_0 S_v r_{n1}}{Q_s} = a_2'$, Eq. (5.2) becomes

$$\frac{dC_i}{dt} = a_2' t^{-r_{n2}} - b C_i + \frac{a_r}{V t^{b_r}} + a_1 (B_1 e^{-B_3 t} + B_2 e^{-B_4 t}) + \frac{D}{V}. \quad (5.4)$$

Following the similar method of deriving Eq. (4.11), the indoor airborne particle concentration is obtained by solving Eq. (5.4) as

$$C_i(t) = e^{-bt} C_i(0) + a_2' e^{-bt} \int_0^t \frac{e^{bt}}{t^{r_{n2}}} dt + \frac{a_r}{V} e^{-bt} \int_0^t \frac{e^{bt}}{t^{b_r}} dt + \quad (5.5)$$

$$\frac{a_1 B_1}{b-B_3} (e^{-B_3 t} - e^{-bt}) + \frac{a_1 B_2}{b-B_4} (e^{-B_4 t} - e^{-bt}) + \frac{D}{V} (1 - e^{-bt}) .$$

Putting Eq. (5.5) back into Eq. (5.3) and integrating with respect to time from 0 to t give the surface particle concentration as

$$\begin{aligned} M(t) = M(0) + \frac{v_{df} C_i(0)}{b} (1 - e^{-bt}) - \frac{a_r}{S_r(1-b_r)} t^{1-b_r} + \\ v_{df} a_2' \int_0^t \left\{ e^{-bt} \left[\int_0^t \frac{e^{b\tau}}{(\tau)^{r_{n2}}} d\tau \right] \right\} dt + \frac{v_{df} a_r}{V} \int_0^t \left\{ e^{-bt} \left[\int_0^t \frac{e^{b\tau}}{\tau^{b_r}} d\tau \right] \right\} dt + \\ \frac{v_{df} a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 t}) - \frac{1}{b} (1 - e^{-bt}) \right] + \frac{v_{df} a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 t}) - \right. \\ \left. \frac{1}{b} (1 - e^{-bt}) \right] + \frac{v_{df} D}{V} t - \frac{v_{df} D}{Vb} (1 - e^{-bt}). \end{aligned} \quad (5.6)$$

Applying the theorem of integration by parts to the 4th and 5th terms on the right hand side of Eq. (5.6) yields

$$\begin{aligned} M(t) = \\ M(0) + \frac{v_{df} C_i(0)}{b} (1 - e^{-bt}) - \frac{a_r}{S_r(1-b_r)} t^{1-b_r} + \frac{v_{df} a_2'}{b} \left[\int_0^t \frac{1}{\tau^{r_{n2}}} dt - \right. \\ \left. e^{-bt} \int_0^t \frac{e^{bt}}{\tau^{r_{n2}}} dt \right] + \frac{v_{df} a_r}{Vb} \left[\int_0^t \frac{1}{\tau^{b_r}} dt - e^{-bt} \int_0^t \frac{e^{bt}}{\tau^{b_r}} dt \right] + \frac{v_{df} a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - \right. \\ \left. e^{-B_3 t} - \frac{1}{b} (1 - e^{-bt}) \right] + \frac{v_{df} a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 t} - \frac{1}{b} (1 - e^{-bt}) \right] \\ \left. \right] + \frac{v_{df} DV}{V} t - \frac{v_{df} DV}{Vb} (1 - e^{-bt}) \\ (1 - e^{-bt}) = M(0) + \frac{v_{df} C_i(0)}{b} - \frac{a_r}{S_r(1-b_r)} t^{1-b_r} + \frac{v_{df} a_2'}{b(1-r_{n2})} t^{1-r_{n2}} + \\ \frac{v_{df} a_r}{Vb(1-b_r)} t^{1-b_r} - \frac{v_{df} C_i(t)}{b} + \frac{v_{df} a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 t}) - \frac{1}{b} (1 - \right. \\ \left. e^{-B_3 t}) \right] + \frac{v_{df} a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 t}) - \frac{1}{b} (1 - e^{-B_4 t}) \right] + \frac{v_{df} D}{V} t . \end{aligned} \quad (5.7)$$

The above models (Eq. (5.5) and Eq. (5.7)) are applicable for the cases where either AIPR or WIPR occurs solely and the cases where AIPR and WIPR occur simultaneously. However, the AIPR in the ventilation duct and the WIPR indoors do not necessarily occur simultaneously. If the WIPR occurs after a period of Δt since the resuspended pathogens in the ventilation duct enter indoors, Eq. (5.4) needs to be modified to

$$\begin{aligned} \frac{dC_i}{dt} = a_2' (t + \Delta t)^{-r_{n2}} - bC_i + \frac{a_r}{V t^{b_r}} + a_1(B_1 e^{-B_3 t} + \\ B_2 e^{-B_4 t}) + \frac{D}{V}, \end{aligned} \quad (5.8)$$

which describes the variation of airborne particle concentration after walking begins.

The corresponding solution for airborne particle concentration is

$$\begin{aligned} C_i(t) = e^{-bt} C_i(0) + a_2' e^{-bt} \int_0^t \frac{e^{bt}}{(t+\Delta t)^{r_{n2}}} dt + \frac{a_r}{V} e^{-bt} \int_0^t \frac{e^{bt}}{t^{b_r}} dt + \\ \frac{a_1 B_1}{b-B_3} (e^{-B_3 t} - e^{-bt}) + \frac{a_1 B_2}{b-B_4} (e^{-B_4 t} - e^{-bt}) + \frac{D}{V} (1 - e^{-bt}), \end{aligned} \quad (5.9)$$

and the corresponding solution for surface particle concentration is

$$\begin{aligned} M(t) = M(0) + \frac{v_{df} C_i(0)}{b} - \frac{a_r}{s_r(1-b_r)} t^{1-b_r} + \frac{v_{df} a_2'}{b(1-r_{n2})} [(t + \Delta t)^{1-r_{n2}} - \\ \Delta t^{1-r_{n2}}] + \frac{v_{df} a_r}{V b(1-b_r)} t^{1-b_r} - \frac{v_{df} C_i(t)}{b} + \frac{v_{df} a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 t}) - \right. \\ \left. \frac{1}{b} (1 - e^{-B_3 t}) \right] + \frac{v_{df} a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 t}) - \frac{1}{b} (1 - e^{-B_4 t}) \right] + \frac{v_{df} D}{V} t. \end{aligned} \quad (5.10)$$

Note that the initial concentration, $C_i(0)$ and $M(0)$ in Eq. (5.9) and Eq. (5.10) will be obtained from Eq. (5.5) and Eq. (5.7), respectively.

If the resuspended pathogens in the duct enter indoors after a period of Δt since the start of WIPR indoors, Eq. (5.4) needs to be modified to

$$\begin{aligned} \frac{dC_i}{dt} = a_2' t^{-r_{n2}} - bC_i + \frac{a_r}{V(t+\Delta t)^{b_r}} + a_1(B_1 e^{-B_3 t} + B_2 e^{-B_4 t}) + \\ \frac{D}{V}, \end{aligned} \quad (5.11)$$

and Eq. (5.3) needs to be modified to

$$\frac{dM}{dt} = C_i v_{df} - \frac{a_r}{s_r(t+\Delta t)^{b_r}}. \quad (5.12)$$

Eq. (5.11) and Eq. (5.12) describe the variation of airborne and surface particle concentrations, respectively, after the resuspended pathogens in the duct enter indoors.

The corresponding solution for airborne particle concentration is

$$C_i(t) = e^{-bt}C_i(0) + a_2' e^{-bt} \int_0^t \frac{e^{bt}}{t^{r_{n2}}} dt + \frac{a_r}{V} e^{-bt} \int_0^t \frac{e^{bt}}{(t+\Delta t)^{b_r}} dt + \frac{a_1 B_1}{b-B_3} (e^{-B_3 t} - e^{-bt}) + \frac{a_1 B_2}{b-B_4} (e^{-B_4 t} - e^{-bt}) + \frac{D}{V} (1 - e^{-bt}), \quad (5.13)$$

and the corresponding solution for surface particle concentration is

$$M(t) = M(0) + \frac{v_{df} C_i(0)}{b} - \frac{a_r}{S_r(1-b_r)} [(t + \Delta t)^{1-b_r} - \Delta t^{1-b_r}] + \frac{v_{df} a_2'}{b(1-r_{n2})} t^{1-r_{n2}} + \frac{v_{df} a_r}{V b(1-b_r)} [(t + \Delta t)^{1-b_r} - \Delta t^{1-b_r}] - \frac{v_{df} C_i(t)}{b} + \frac{v_{df} a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 t}) - \frac{1}{b} (1 - e^{-B_3 t}) \right] + \frac{v_{df} a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 t}) - \frac{1}{b} (1 - e^{-B_4 t}) \right] + \frac{v_{df} D}{V} t \quad (5.14)$$

Note that the initial concentration, $C_i(0)$ and $M(0)$ in Eq. (5.13) and Eq. (5.14) will be obtained from Eq. (5.5) and Eq. (5.7), respectively.

It is obvious that the role of each source on airborne and surface concentrations could be clearly identified based on the derived models. For example, the airborne concentration models (Eq. (5.5), Eq. (5.9) and Eq. (5.13)) consist of six terms. The first term accounts for the effect of initial airborne concentration. The second and third terms account for the effect of AIPR in the ventilation duct and WIPR indoors, respectively. The fourth and fifth terms account for the effect of outdoor concentration. The sixth term accounts for the effect of indoor constant emission source. The indoor particle loss mechanisms (e.g., deposition and ventilation) reflected by b affect all six terms in the way of exponential function. The airborne concentration is resultant from the superposition of initial concentration, AIPR, WIPR, outdoor concentration and indoor constant emission source under the effect of these loss mechanisms. Hence, based on the above models, the relative contribution of AIPR and WIPR towards indoor airborne and surface concentrations under a certain ventilation, building and occupancy conditions could be clearly identified.

It should be noted that when the outdoor concentration C_o is constant, that is, $C_o = B_1 + B_2$, the terms accounting for the effect of outdoor source in the above airborne and surface particle concentration models will be changed to $\frac{a(B_1+B_2)}{b}(1 - e^{-bt})$ and $\frac{v_{df}a(B_1+B_2)}{b}t$, respectively.

5.3 Model validation

The model validation about the case with AIPR in the ventilation duct is impossible due to the lacking of relevant data for the time being and is left for future study. The model validation about the case with WIPR indoors is conducted by comparing existing experimental data [15, 18] to model predictions.

The study of Qian and Ferro [18] measured the airborne particle ($0.4 - 10 \mu\text{m}$) concentration variation in a full-scaled chamber where a participant performed prescribed activities on the seeded carpet. The participant firstly walked on the carpet for 5 minutes, followed by sitting for 20 minutes, and then walked for 5 minutes again followed by leaving the chamber. The airborne concentration profiles for $2 - 3 \mu\text{m}$ and $4 - 5 \mu\text{m}$ particles are selected for validation. A HEPA filter was installed for the chamber ventilation and the outdoor airborne particles did not enter the chamber during the measurements as mentioned by the authors. The test dust was seeded onto the carpet to a mass concentration of 20 g/m^2 based on which the number concentrations of $2 - 3 \mu\text{m}$ and $4 - 5 \mu\text{m}$ particles can be estimated in terms of the size distribution (Figure 3.2) of test dust and the particle density (2650 kg/m^3). The

surface mass concentrations for 2 – 3 μm and 4 – 5 μm particles are ($20 \times 0.13 = 2.6 \text{ g/m}^2$) and ($20 \times 0.2 = 4 \text{ g/m}^2$), respectively. The RH in the experiments was 31.7%. The particle resuspension area is 5.95 m^2 . To determine the resuspension rate for the WIPR, the resuspension rate ($R(t) = 2.25t^{-0.58}$ as shown in Table 4.1) of the carpet/ PM_{10} case at the walking rate of 132 steps/min under the RH of 82% in Chapter 4 is used as the reference. In the reference case, the resuspension area is 0.2 m^2 and the surface mass concentration is 1.75 g/m^2 . Based on the study in Chapter 4, the normalized resuspension rate for the case under the RH of 31.7% is assumed to be 5 ~ 6 times of that under the RH of 82%. The normalized resuspension rate of PM_{10} was about 2.5 times of $\text{PM}_{2.5}$ and the resuspension is more significant for larger particles according to Chapter 4. It is assumed that the normalized resuspension rates for the cases of 2 – 3 μm and 4 – 5 μm particles are (0.4 ~ 0.6) and (0.8 ~ 1.0) times of that of PM_{10} , respectively. Hence, the power law coefficient of resuspension rate for 2 – 3 μm particles is estimated to range from $[2.25 \times 5 \times 0.4 \times 2.6 \times 5.95 / (0.2 \times 1.75) = 198.9]$ to $[2.25 \times 6 \times 0.6 \times 2.6 \times 5.95 / (0.2 \times 1.75) = 358.0]$ and the resuspension rate for 2 – 3 μm particles varies from $R(t) = 198.9t^{-0.58}$ to $R(t) = 358.0t^{-0.58}$ in the unit of $\mu\text{g/s}$. The power law coefficient of resuspension rate for 4 – 5 μm particles is approximated to range from $[2.25 \times 5 \times 0.8 \times 4 \times 5.95 / (0.2 \times 1.75) = 612.0]$ to $[2.25 \times 6 \times 1.0 \times 4 \times 5.95 / (0.2 \times 1.75) = 918.0]$ and the resuspension rate for 4 – 5 μm particles varies from $R(t) = 612.0t^{-0.58}$ to $R(t) = 918.0t^{-0.58}$ in the unit of $\mu\text{g/s}$. In view of the measured airborne concentration was in the unit of $\#/s$, the resuspension rate is further divided by the mass of a single particle (m_p) to covert the unit of $\mu\text{g/s}$ to $\#/s$. The average diameters, 2.5 and 4.5 μm , are used to represent 2 – 3 μm and 4 – 5 μm particles, respectively. m_p for 2.5 μm and 4.5 μm spherical particles are

$2.17 \times 10^{-5} \mu\text{g}$ and $12.64 \times 10^{-5} \mu\text{g}$, respectively. Correspondingly, the resuspension rates in the unit of #/s vary from $R(t) = 9.2 \times 10^6 t^{-0.58}$ (lower resuspension rate) to $R(t) = 1.7 \times 10^7 t^{-0.58}$ (upper resuspension rate) and from $R(t) = 4.8 \times 10^6 t^{-0.58}$ (lower resuspension rate) to $R(t) = 7.3 \times 10^6 t^{-0.58}$ (upper resuspension rate) for $2 - 3 \mu\text{m}$ and $4 - 5 \mu\text{m}$ particles, respectively.

The study of Ferro et al. [15] measured the airborne particle ($2.5 - 5 \mu\text{m}$) concentration in a real house following a series of activities (one person dancing on a rug for 15 minutes, one person walking on a rug for 15 minutes and one person dancing on a wood floor for 18 minutes). The outdoor concentration slightly varied during the experiment and, thus, was set to be a constant value of $1.85 \mu\text{g}/\text{m}^3$ for modeling. The flooring area is 104 m^2 and the walking area is assumed to range from $80 \sim 104 \text{ m}^2$. The initial particle surface concentration, $M(0)$, was not provided in the article. Thatcher et al. [202] measured the surface concentration on the rug in a real house to be $1.1 \text{ g}/\text{m}^2$. It is assumed that $M(0) = 0.8 \sim 1.5 \text{ g}/\text{m}^2$ on the rug in the study of Ferro et al. [15]. Considering that carpet generally has the higher potential of accumulating dust than wood floor indoors, it is assumed that the surface concentration is $1/4 \sim 1/6$ of that for the rug; that is, $M(0) = 0.133 \sim 0.375 \text{ g}/\text{m}^2$ for the wood floor. The fraction of $2.5 - 5 \mu\text{m}$ particles in the dust was estimated to range from 15% to 25% [203]. As a result, the surface mass concentrations of $2.5 - 5 \mu\text{m}$ particles range from $0.12 \text{ g}/\text{m}^2$ to $0.375 \text{ g}/\text{m}^2$ and from $0.02 \text{ g}/\text{m}^2$ to $0.094 \text{ g}/\text{m}^2$ for the rug and wood flooring, respectively. The RH is not given in the study. However, it is noted that the experiments were conducted in April in an apartment located at Redwood city and the average RH during April in Redwood city was 80% [204]. For

walking and dancing on the rug, the resuspension rate ($R(t) = 2.25t^{-0.58}$ as shown in Table 4.1) of the carpet/PM₁₀ case at the walking rate of 132 steps/min under the RH of 82% from Chapter 4 is used as the reference. The power law coefficient of resuspension rate for walking on the rug is estimated to range from $[2.25 \times 0.12 \times 80 / (0.2 \times 1.75) = 61.7]$ to $[2.25 \times 0.375 \times 104 / (0.2 \times 1.75) = 250.7]$ and the corresponding resuspension rate varies from $R(t) = 61.7t^{-0.58}$ (lower resuspension rate) to $R(t) = 250.7t^{-0.58}$ (upper resuspension rate) in the unit of $\mu\text{g/s}$. The dancing activity is treated to be a more vigorous walking and thus should correspond to a more significant resuspension. It is assumed that the resuspension rate for dancing on the rug is 3~4 times of that for walking on the rug. As a result, the resuspension rate for dancing on the rug varies from $R(t) = 185.1t^{-0.58}$ (lower resuspension rate) to $R(t) = 1002.9t^{-0.58}$ (upper resuspension rate) in the unit of $\mu\text{g/s}$. For dancing on the wood floor, the resuspension rate ($R(t) = 0.68t^{-0.42}$ as shown in Table 4.1) of the wood/PM₁₀ case at the walking rate of 132 steps/min under the RH of 82% from Chapter 4 is used as the reference. It is assumed that the normalized resuspension rate for dancing on the wood floor is 2~3 times of that for walking on the wood floor. Hence, the power law coefficient of the resuspension rate for dancing on the wood floor ranges from $[0.68 \times 0.02 \times 80 \times 2 / (0.2 \times 2.26) = 4.8]$ to $[0.68 \times 0.094 \times 104 \times 3 / (0.2 \times 2.26) = 44.1]$ and the corresponding resuspension rate varies from $R(t) = 4.8t^{-0.42}$ (lower resuspension rate) to $R(t) = 44.1t^{-0.42}$ (upper resuspension rate) in the unit of $\mu\text{g/s}$. The parameters required for modeling are listed in Table 5.2. The comparison between the experimental data and model predictions are given in Figure 5.1. The model predictions are based on the lower and upper resuspension rates, respectively.

Table 5.2 Parameters used for model predictions during the validation.

Parameters	Meaning	Studies for validation	
		Qian and Ferro [18]	Ferro et al. [15]
α_a (1/s)	Air exchange rate	1.11×10^{-4}	1.28×10^{-4}
p_c	Penetration through building shell	—	1
R_r	Fraction of recirculated air	0	—
η_r	Filter efficiency	1	—
p_b	Penetration through bend(s)	—	—
d_v	Deposition loss in the duct	—	—
v_{df} (m/s)	Deposition velocity onto floor	1.0×10^{-3} (2.5 μm) 2.5×10^{-3} (4.5 μm)	7.0×10^{-4}
v_{dw} (m/s)	Deposition velocity onto wall	9.0×10^{-5} (2.5 μm) 3.0×10^{-5} (4.5 μm)	1.0×10^{-5}
v_{dc} (m/s)	Deposition velocity onto ceiling	5.0×10^{-6} (2.5 μm) 1.0×10^{-6} (4.5 μm)	6.0×10^{-7}
A_f (m ²)	Area of floor	17.86	104
A_w (m ²)	Area of wall	52.09	102
A_c (m ²)	Area of ceiling	17.86	104
V (m ³)	Volume of indoor space	54.48	260
β_b (m ³ /s)	Breathing rate of occupants	2.83×10^{-4}	2.83×10^{-4}
n_p	Number of occupants	1	1
$C_i(0)$ (#/m ³)	Initial indoor airborne concentration	0	19.86 [#]
$M(0)$ (μg/m ²)	Initial indoor surface concentration for resuspension	2.6×10^6 (2.5 μm) 4.0×10^6 (4.5 μm)	$1.2 \times 10^5 \sim 3.75 \times 10^5$ (rug) $2.0 \times 10^4 \sim 9.4 \times 10^4$ (wood)
C_o (#/m ³)	Outdoor concentration	—	$1.85(e^{0t} + e^{0t})^{\#}$
R (#/s)	Resuspension rate	$(5.5 \times 10^6 \sim 1.9 \times 10^7)t^{-0.58}$ (2.5 μm) $(3.4 \times 10^6 \sim 8.0 \times 10^7)t^{-0.58}$ (2.5 μm)	$(185.1 \sim 1002.9)t^{-0.58}$ (dancing on rug) [†] $(61.7 \sim 250.7)t^{-0.58}$ (walking)

		$10^6)t^{-0.58}$ (4.5 μm)	on rug) [‡]
			(4.8~44.1) $t^{-0.42}$ (dancing on
			wood) [‡]
E (#/s)	Emission rate	—	—

†: The breathing rate is obtained from the study of Kolwaski [12].

#: The unit is $\mu\text{g}/\text{m}^3$ for the case from the study of Ferro et al. [15].

‡: The unit is $\mu\text{g}/\text{s}$ for the case from the study of Ferro et al. [15].

Figure 5.1 The comparison between the model predictions and experimental data from the studies of (a) Qian and Ferro [18] (2.5 μm particles), (b) Qian and Ferro [18] (4.5 μm particles), and (c) Ferro et al. [15]. Note that for the parameters not given in the original studies, reference values were firstly found from the previous literatures or Chapter 4. The reference values were generally varied by $\pm 20\%$ to account for their potential uncertainty during modeling.

It is shown in Figure 5.1 (a) and (b) that the model predictions based on lower and upper resuspension rate well cover the experimental data and describe the variation of airborne concentration; that is, the concentration quickly increases during the walking period due to the overwhelming effect of WIPR and declines during the non-walking period due to the particle loss mechanisms. The increase of airborne concentration for 2.5 μm particles is larger than that for 4.5 μm particles due to the fact that the initial surface concentration is larger for 2.5 μm particles. This is also reflected by the larger resuspension rate of 2.5 μm particles than that of 4.5 μm particles shown in Table 5.2. Figure 5.1 (c) also shows that the model predictions reasonably cover the experimental data. The airborne particle concentration during the activity period increases most significantly for dancing on the rug, followed by walking on the rug

and dancing on the wood floor. This corresponds to the most significant resuspension induced by dancing on the rug followed by walking on the rug and dancing on the wood floor as shown in Table 5.2.

5.4 Conclusions

The model of airborne particle concentration dynamics in the ventilation duct with AIPR (Chapter 3) and the power-law resuspension rate for WIPR indoors (Chapter 4) were substituted into the two-compartment mass balance models to develop a set of indoor airborne and surface particle concentration models. The contributions of the potential resuspension processes (AIPR and WIPR) towards indoor particle dynamics could be clearly identified based on the developed models. The developed models were validated against the existing experimental data and a good agreement has been found. These models provide a basis for the pathogen exposure estimation and thus the infection risk assessment in the following chapter.

Chapter 6 Risk Assessment Scheme for Infection Transmission Indoors Considering Resuspension Processes

6.1 Introduction

Risk assessment is one of important measures towards controlling and managing infection transmission. Accurate exposure analysis serves as the basis for the development of an appropriate risk assessment scheme. The developed models in Chapter 5 can be used to construct the exposure analysis and thus the risk assessment. The capability of predicting the effect of resuspension on airborne and surface concentrations in the models of Chapter 5 allows the effect of resuspension on infection transmission to be considered in a corresponding risk assessment scheme.

6.2 Exposure analysis model

Since inhalational infection risk is generally the main component of overall infection risk [21], only inhalational exposure is considered here. During the estimation of inhalational exposure, persistence of pathogens in the environment needs to be considered. As reviewed in Chapter 2, persistence of pathogens can be expressed by the fraction of pathogens survived after a certain period of time, p_{fs} , in the exponential function (Eq. (2.16)). The inhalational exposure during a period of T_e can be calculated as

$$I = \beta_b p_{fi} p_{fs} \int_0^{T_e} C_i(t) dt . \quad (6.1)$$

p_{fi} is the inhalability parameter accounting for the real exposure to pathogens, considering not every exposed pathogen could enter the head, either through nasal or

oral passages. p_{fi} is estimated based on the aerodynamic diameter, d_{ae} , of pathogens as [205]

$$p_{\text{fi}} = 1 - 0.15[\log_{10}(1 + d_{\text{ae}})]^2 - 0.10\log_{10}(1 + d_{\text{ae}}). \quad (6.2)$$

For the pathogens of extremely low decay rate (extremely persistent) such as *B. anthracis*, $p_{\text{fs}} \approx 1$ for the period of hundreds of hours and thus Eq. (6.1) can be approximated by

$$I = \beta_{\text{b}} p_{\text{fi}} \int_0^{T_{\text{e}}} C_{\text{i}}(t) dt \quad (6.3)$$

In order to estimate the inhalational exposure, the airborne concentration models (Eq. (5.5), Eq. (5.9) and Eq. (5.13)) in Chapter 5 are substituted into the integral of Eq. (6.1), $\int_0^{T_{\text{e}}} C_{\text{i}}(t) dt$. Corresponding to Eq. (5.5),

$$\begin{aligned} \int_0^{T_{\text{e}}} C(t) dt &= \frac{C_{\text{i}}(0)}{b} + \frac{a_2'}{b(1-r_{\text{n}2})} T_{\text{e}}^{1-r_{\text{n}2}} + \frac{a_{\text{r}}}{vb(1-b_{\text{r}})} T_{\text{e}}^{1-b_{\text{r}}} - \frac{C_{\text{i}}(T_{\text{e}})}{b} + \\ &\frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_{\text{e}}}) - \frac{1}{b} (1 - e^{-B_3 T_{\text{e}}}) \right] + \frac{a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_{\text{e}}}) - \right. \\ &\left. \frac{1}{b} (1 - e^{-B_4 T_{\text{e}}}) \right] + \frac{D}{V} T_{\text{e}} = \frac{M(T_{\text{e}}) - M(0) + \frac{a_{\text{r}}}{S_{\text{r}}(1-b_{\text{r}})} T_{\text{e}}^{1-b_{\text{r}}}}{v_{\text{df}}}, \end{aligned} \quad (6.4)$$

and thus the exposure estimation is

$$\begin{aligned} I &= \beta_{\text{b}} p_{\text{fi}} p_{\text{fs}} \left\{ \frac{C_{\text{i}}(0)}{b} + \frac{a_2'}{b(1-r_{\text{n}2})} T_{\text{e}}^{1-r_{\text{n}2}} + \frac{a_{\text{r}}}{vb(1-b_{\text{r}})} T_{\text{e}}^{1-b_{\text{r}}} - \frac{C_{\text{i}}(T_{\text{e}})}{b} + \right. \\ &\frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_{\text{e}}}) - \frac{1}{b} (1 - e^{-B_3 T_{\text{e}}}) \right] + \frac{a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_{\text{e}}}) - \right. \\ &\left. \frac{1}{b} (1 - e^{-B_4 T_{\text{e}}}) \right] + \frac{D}{V} T_{\text{e}} \left. \right\} = \beta_{\text{b}} p_{\text{fi}} p_{\text{fs}} \left[\frac{M(T_{\text{e}}) - M(0) + \frac{a_{\text{r}}}{S_{\text{r}}(1-b_{\text{r}})} T_{\text{e}}^{1-b_{\text{r}}}}{v_{\text{df}}} \right]. \end{aligned} \quad (6.5)$$

Corresponding to Eq. (5.9),

$$\begin{aligned}
\int_0^{T_e} C(t)dt &= \frac{C_i(0)}{b} + \frac{a_2'}{b(1-r_{n2})} [(T_e + \Delta t)^{1-r_{n2}} - \Delta t^{1-r_{n2}}] + \\
&\frac{a_r}{vb(1-b_r)} T_e^{1-b_r} - \frac{C_i(T_e)}{b} + \frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_e}) - \frac{1}{b} (1 - \right. \\
&e^{-B_3 T_e}) \left. \right] + \frac{a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_e}) - \frac{1}{b} (1 - e^{-B_4 T_e}) \right] + \frac{D}{V} T_e = \\
&\frac{M(T_e) - M(0) + \frac{a_r}{S_r(1-b_r)} T_e^{1-b_r}}{v_{df}},
\end{aligned} \tag{6.6}$$

and thus the exposure estimation is

$$\begin{aligned}
I &= \beta_b p_{fi} p_{fs} \left\{ \frac{C_i(0)}{b} + \frac{a_2'}{b(1-r_{n2})} [(T_e + \Delta t)^{1-r_{n2}} - \Delta t^{1-r_{n2}}] + \right. \\
&\frac{a_r}{vb(1-b_r)} T_e^{1-b_r} - \frac{C_i(T_e)}{b} + \frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_e}) - \frac{1}{b} (1 - \right. \\
&e^{-B_3 T_e}) \left. \right] + \frac{a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_e}) - \frac{1}{b} (1 - e^{-B_4 T_e}) \right] + \frac{D}{V} T_e \left. \right\} = \\
&\beta_b p_{fi} p_{fs} \left[\frac{M(T_e) - M(0) + \frac{a_r}{S_r(1-b_r)} T_e^{1-b_r}}{v_{df}} \right].
\end{aligned} \tag{6.7}$$

Corresponding to Eq. (5.13),

$$\begin{aligned}
\int_0^{T_e} C(t)dt &= \frac{C_i(0)}{b} + \frac{a_2'}{b(1-r_{n2})} T_e^{1-r_{n2}} + \frac{a_r}{vb(1-b_r)} [(T_e + \\
&\Delta t)^{1-b_r} - \Delta t^{1-b_r}] - \frac{C_i(T_e)}{b} + \frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_e}) - \frac{1}{b} (1 - \right. \\
&e^{-B_3 T_e}) \left. \right] + \frac{a_1 B_2}{b-B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_e}) - \frac{1}{b} (1 - e^{-B_4 T_e}) \right] + \frac{D}{V} T_e = \\
&\frac{M(T_e) - M(0) + \frac{a_r}{S_r(1-b_r)} [(T_e + \Delta t)^{1-b_r} - \Delta t^{1-b_r}]}{v_{df}},
\end{aligned} \tag{6.8}$$

and thus the exposure estimation is

$$\begin{aligned}
I &= \beta_b p_{fi} p_{fs} \left\{ \frac{C_i(0)}{b} + \frac{a_2'}{b(1-r_{n2})} T_e^{1-r_{n2}} + \frac{a_r}{vb(1-b_r)} [(T_e + \Delta t)^{1-b_r} - \right. \\
&\Delta t^{1-b_r}] - \frac{C_i(T_e)}{b} + \frac{a_1 B_1}{b-B_3} \left[\frac{1}{B_3} (1 - e^{-B_3 T_e}) - \frac{1}{b} (1 - e^{-B_3 T_e}) \right] +
\end{aligned} \tag{6.9}$$

$$\frac{a_1 B_2}{b - B_4} \left[\frac{1}{B_4} (1 - e^{-B_4 T_e}) - \frac{1}{b} (1 - e^{-B_4 T_e}) \right] + \frac{D}{V} T_e \} =$$

$$\beta_b p_{fi} p_{fs} \left[\frac{M(T_e) - M(0) + \frac{a_r}{s_r(1-b_r)} [(T_e + \Delta t)^{1-b_r} - \Delta t^{1-b_r}]}{v_{df}} \right].$$

It should be noted that in the case without WIPR, $\int_0^{T_e} C(t) dt = \frac{M(T_e) - M(0)}{v_{df}}$, and thus

$$I = \beta_b p_{fi} p_{fs} \left[\frac{M(T_e) - M(0)}{v_{df}} \right]. \quad (6.10)$$

That is, the inhalational exposure is directly proportional to the pathogen surface concentration. This suggests that the exposure estimation can be performed on the basis of the measurement of surface concentration, which is of practical purpose for post-epidemic or post-attack responses.

6.3 Dose response model

As reviewed in Chapter 2, the infection probability could be estimated by substituting the exposure estimation, I , into the exponential (Eq. (2.17)) or beta-Poisson (Eq. (2.18)) dose-response models with knowledge of the fitting parameters accounting for the infectivity of pathogen and the pathogen-host interactions. The models are not repeated here.

6.4 Case Study

Two cases are studied: (1) pathogens are covertly dosed onto the floor of ventilation duct when the ventilation is off and some of them are resuspended and transported into indoor environment when the ventilation system is running again; (2) pathogens

are placed onto the indoor floor and some of them are resuspended due to human walking. The first case is further divided into two sub-cases: the one without WIPR and the one with WIPR. The representative BW agent, *B. anthracis*, is considered as the pathogen in the case study. *B. anthracis* is a Gram-positive, spore-forming bacillus with the approximate size of $1\ \mu\text{m} \times 5\ \mu\text{m}$ [144]. Although there are three types of anthrax (inhalational anthrax, cutaneous anthrax and gastrointestinal anthrax) in terms of exposure pathways, the inhalational anthrax is the most life-threatening one with the mortality rate as high as 90% - 99% if untreated [206]. This reinforces the importance of inhalational exposure analysis for *B. anthracis*. As introduced in Chapter 2, the exponential dose response model is suitable for *B. anthracis* (Eq. (2.17)).

6.4.1 Case 1

In this case, 10 grams of *B. anthracis* spores are covertly dosed onto the duct floor when the ventilation is off. The initial indoor airborne and surface pathogen concentrations are zero. There are 3 occupants indoors with a breathing rate of $0.000283\ \text{m}^3/\text{s}$ each. The fraction of recirculated air, R_r , is set to be 0.8 [132]. The ventilation duct is made of plastic and has the cross-sectional dimension of $0.25\ \text{m}$ (W) $\times$ $0.25\ \text{m}$ (H) [132]. The air exchange rate is set to be $5\ \text{h}^{-1}$ corresponding to the flow rate of $800\ \text{m}^3/\text{hr}$ in the ventilation duct [207]. This means that the free stream velocity in the ventilation duct is about $3.6\ \text{m/s}$. In order to calculate the normalized resuspension rate for the AIPR and deposition loss in the duct, it is necessary to know the friction velocity of turbulent airflow in the duct. It is assumed that the relationship between the friction velocity and free stream velocity in Chapter 3 also holds in this

case, that is, $u^* = 0.0710U_\infty - 0.0056$. The normalized resuspension rate for AIPR is obtained as the average of the emp1 (Eq. (2.11)) from [116] and the model II-A (Eq. (2.13)) from [98]. The parameters needed for calculating the normalized resuspension rate are listed in Table 6.1. It is assumed that both dosed agents and recirculated agents will go through 5 bends before they enter indoors. The penetration coefficient of bend (p_b) is approximated to be 100% for the considered airflow condition and size of agent [131]. The duct lengths from the agent dosing location and the air outlet to the air supply intake are assumed to be 20 m. An ASHARE 40% filter of the efficiency of 0.8 [130] for 3 μm particles is installed in the ventilation system. The indoor flooring material is carpet and the particle resuspension area (walking area) is assumed to be 20% of the total flooring area.

Table 6.1 Parameters for calculating the normalized resuspension rate of AIPR.

Parameters	Meaning	Unit	Value	Source
d_p	Particle diameter	μm	3	[144]
A_{132}	Hamaker constant	J	$7.12 \times 10^{-20\dagger}$	[98]
u^*	Friction velocity	m/s	0.247	Chapter 3
ρ_p	Particle density	kg/m^3	1200	[32]
ρ_a	Air density	kg/m^3	1.2	[78]
σ_1	Surface roughness	μm	5	[32]

$\dagger$: $A_{132} = \sqrt{A_{11}A_{22}}$, where $A_{11} = 6.5 \times 10^{-20}$ J and $A_{22} = 7.8 \times 10^{-20}$ J are the Hamaker constant of particle and surface, respectively [98].

Two sub-cases are considered: (1) there is no WIPR indoors during the 5-hr period modeled (Sub-case 1); (2) WIPR occurs 4 hrs after the dosed spores enter indoors and lasts for 1 hr (Sub-case 2). On average, there is one occupant walking at the medium

rate (108 steps/min) within the 1-hr walking period. The indoor RH is set to be 40%. The surface particle concentration just before the initiation of walking is calculated to be $1.054 \times 10^{-5} \text{ g/m}^2$ ($621502 \text{ \#/m}^2$) from the modeling of the first sub-case. The resuspension rate for the carpet/PM₁₀ case at the waking rate of 108 steps/min and the RH of 82% in Chapter 4, i.e., $R(t) = 0.96t^{-0.49}$ in the unit of $\mu\text{g/s}$, serves as the reference. As suggested in Chapter 4, the resuspension rate for the case of RH=40% is about 3.5 times of RH=82%. As a result, the power law coefficient of the resuspension rate is estimated to be $[3.5 \times \frac{0.96}{0.2 \times 2.75} \times (12.8 \times 1.054 \times 10^{-5})/m_p = 49]$. m_p (μg) is the mass of a single particle and $m_p = 1.696 \times 10^{-5} \mu\text{g}$ for the considered *B. anthracis*. Hence, the power law resuspension rate of WIPR in Sub-case 2 is $R(t) = 49t^{-0.49}$ in the unit of $\text{\#/s}$. The parameters used for calculating the particle concentrations and infection probability are summarized in Table 6.2.

Table 6.2 Parameters required by modeling for the case study.

Parameter	Meaning	Case 1	Case 2
α_a (1/s)	Air exchange rate	1.39×10^{-3}	1.39×10^{-3}
p_c	Penetration through building shell	–	–
R_r	Fraction of recirculated air	0.8	0.8
η_r	Filter efficiency	0.8	0.8
p_b	Penetration through bend(s)	1	1
d_v	Deposition loss in the duct	0.98	0.98
v_{df} (m/s)	Deposition velocity onto floor	2.0×10^{-3}	2.0×10^{-3}
v_{dw} (m/s)	Deposition velocity onto wall	6.0×10^{-5}	6.0×10^{-5}
v_{dc} (m/s)	Deposition velocity onto ceiling	3.0×10^{-6}	3.0×10^{-6}
A_f (m ²)	Area of floor	64	64
A_w (m ²)	Area of wall	80	80
A_c (m ²)	Area of ceiling	64	64

V (m ³)	Volume of indoor space	160	160
β_b (m ³ /s)	Breathing rate of occupants	2.83×10^{-4}	2.83×10^{-4}
n_p	Number of occupants	3	3
$C_i(0)$ (#/m ³)	Initial indoor airborne concentration	0	0
$M(0)$ (#/m ²)	Initial indoor surface concentration for resuspension	0	4.61×10^9
C_o (#/m ³)	Outdoor concentration	0	0
Λ (1/s)	Normalized resuspension rate for AIPR	$1.3 \times 10^{-3}t^{-0.97}$	–
R (#/s)	Resuspension rate WIPR	$49t^{-0.49}$	$3601081t^{-0.49}$
E (#/s)	Emission rate	–	–
p_{fi}	Inhalability parameter	1	1
γ_d (1/s)	Pathogen decay rate in air	$2.27 \times 10^{-8\dagger}$	$2.27 \times 10^{-8\dagger}$
r_i	Virulence coefficient of pathogen	$7.15 \times 10^{-6\dagger}$	$7.15 \times 10^{-6\dagger}$
ρ_p (kg/m ³)	Pathogen density	1200 ^{&}	1200 ^{&}

†: The data is from Hong et al. [21].

&: The data is from Krauter and Biermann [32].

The airborne and surface pathogen concentrations and infection probability for Sub-case 1 and Sub-case 2 are shown in Figure 6.1 and Figure 6.2, respectively. For Sub-case 2, only the data within the 1-hr walking period (4 – 5 hr) is shown in Figure 6.2, because the concentrations and infection probability of Sub-case 2 are the same as Sub-case 1 for the non-walking period. But the data of Sub-case 1 during 4 – 5 hr is added in Figure 6.2 for comparison purposes.

Figure 6.1 The modeling results for Sub-case 1: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability.

In Sub-case 1, the airborne pathogen concentration increases for up to about 0.005 hr and then declines quickly for up to about 2 hr followed by a very slow decrease afterwards. The airborne pathogen concentration only decreases by one half (from 1300 #/m³ to 530 #/m³) for the period of 2 – 5 hr, suggesting the prolonged inhalational exposure for occupants. These phenomena are related to the fact that the AIPR decays as time in the manner of power law relation: the decay rate of

resuspension rate decreases as time. The surface pathogen concentration increases all the way through 5 hrs due to the effect of deposition. The surface concentration increases very quickly before 0.5 hr followed by a slow increase corresponding to the small airborne concentration then. The infection probability increases fast as time within the exposure period of 0.5 hr and increases relatively slow afterwards. This emphasizes the importance of early evacuation action against the bioterrorist attack. The variation pattern of infection probability (Figure 6.1 (b)) is similar to that of surface concentration. This is due to that the pathogen exposure is related to the surface concentration variation in the case without walking as shown in the exposure analysis model, Eq. (6.10).

Figure 6.2 The modeling results for Sub-case 2: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability. The results of Sub-case 1 are added for comparison purposes.

It is shown in Figure 6.2 (a) that the WIPR increases the airborne pathogen concentration by less than 1% and decreases the surface pathogen concentration by less than 0.1% compared to Sub-case 1. The infection probability of Sub-case 2 is almost overlapping with that of Sub-case 1, suggesting the negligible effect of WIPR on infection transmission in this case. This is because the number of pathogens resuspended is significantly smaller than the number of airborne pathogens due to the limited surface pathogen concentration ($60/\text{cm}^2$) on the floor. If both a larger amount of pathogen (e.g., 10 kg) and a later walking initiation time (e.g., 25 hrs) apply, the effect of WIPR on infection transmission will become significant.

6.4.2 Case 2

In this case, 10 grams of *B. anthracis* spores are uniformly released onto the floor of a mechanically ventilated room, some of which are subsequently resuspended by human walking. The specifications of the room are listed in Table 6.2. Correspondingly, the initial surface pathogen concentration is $M(0) = 4.61 \times 10^9 \text{ \#/m}^2$. The initial airborne pathogen concentration is $C_i(0) = 0 \text{ \#/m}^3$. It is assumed that there is averagely one occupant walking indoors during a period of 4 hrs. The same walking condition as above is applied here (i.e., carpet flooring, medium walking rate (108 steps/min), RH=40% and 12.8 m^2 walking area). Hence, the power law coefficient of resuspension rate is estimated to be $[3.5 \times \frac{0.96}{0.2 \times 2.75} \times (12.8 \times \frac{10}{12.8}) / m_p = 3601081]$ and the power law resuspension rate for WIPR is $R(t) = 3601081 t^{-0.49}$ in the unit of $\text{\#/s}$. All other parameters are the same as above and listed in Table 6.2. The modeling results are shown in Figure 6.3.

Figure 6.3 The modeling results for Case 2: (a) the variation of airborne and surface pathogen concentrations; (b) the variation of infection probability.

It is shown that the WIPR increases the indoor airborne pathogen concentration to the peak level of $5.7 \times 10^5 \text{ \#/m}^3$ after about 0.11 hr followed by the continuous decay. Corresponding to the power law decrease of resuspension rate, the decrease of airborne concentration since 0.11 hr becomes slower and slower. The airborne pathogen concentrations at 2 hr, 3 hr and 4 hr are $1.50 \times 10^5 \text{ \#/m}^3$, $1.21 \times 10^5 \text{ \#/m}^3$ and $1.05 \times 10^5 \text{ \#/m}^3$, respectively. It could be expected that an approximate steady state for the indoor airborne concentration could be reached, if the indoor walking activity persists for longer period of time (e.g., 10 hours). This suggests that the WIPR could contribute to prolong occupants' exposure to harmful pathogens. The surface pathogen concentration decreases by 1.5% after 4 hrs, showing the depletion effect of walking in the pathogens on the floor.

The infection probability increases very quickly within the first 0.5 hr followed by a much slower increase, consistent with the relatively high concentration within the first 0.5 hr. This means that early identification of the bioterrorist attack and evacuation of occupants are critical for effectively mitigating the attack. After 2-hr exposure, the infection probability is nearly 1, showing the strong capability of the WIPR to cause infection. As a whole, the WIPR has the potential to cause both prolonged exposure and high infection risk in the considered case.

It should be noted that the deposited spores may interact (e.g., coagulation) with the existing dust on the floor, which may affect the resuspension rate for the spores. However, this consideration is beyond the scope of this work and will be left as a future study.

6.5 Conclusions

In this chapter, a set of exposure analysis models was developed based on the concentration models of Chapter 5. A risk assessment scheme of infection transmission was proposed by integrating the exposure analysis models into the dose response model. This scheme is capable of quantifying the effect of the potential pathogen resuspension processes on indoor infection transmission, which was illustrated by the case studies on the bioterrorist attacks. In the case about ventilation systems-based attack, the AIPR in the duct served to prolong occupants' exposure to BW pathogens. In this case, the WIPR could significantly affect infection probability only if a large amount of pathogens were dosed and the walking started long time after the dosed pathogens enter indoors so that there were enough pathogens on the floor for the WIPR. In the case that pathogens were placed on the indoor floor, the

WIPR has the potential to cause both prolonged exposure and high infection risk. Early identification of the bioterrorist attack and evacuation of occupants were found to be critical for effectively mitigating the attack in this case.

Chapter 7 Development of Mean Adhesion Force Model

7.1 Introduction

As described in Chapter 2, the current theoretical AIPR models need to be improved for the potential application in exposure analysis in the future. As the first step, the current capability of modeling particle-surface adhesion forces needs to be enhanced, which will be done in this and next chapters.

When a particle lays on a surface, deformation of particle and surface would occur due to the adhesion force and elasticity of the system. The contact between the particle and surface has a finite area rather than an infinitely small spot. However, if the surface is rough, the existence of asperities makes the actual contact area smaller than the nominal one corresponding to the smooth contact. Hence, in combination with the roughness, the deformation would influence the actual contact area between the particle and surface, which would conversely influence the particle-surface adhesion. Beach et al. [208] suggests that the neglecting of the elastic deformation effect in the previous models [56-58] could have led to substantial inaccuracy in their predictions.

In applying the concept of surface roughness, it should be recognized that there is a wide distribution of roughness scales for real surfaces, which is phenomenally reflected by the fact that the measured roughness is related to the scan length (size) of the measurement methodology employed [209, 210]. It means that multiple roughness scales could co-exist for a single surface. This concept has been initially proposed by

Archard [211], who suggests that the roughness of surface consisted of smaller protuberances superposed on the larger protuberances and even larger protuberances. This actually describes the characteristics of fractal geometry before the fractal theory is developed. Many real surfaces are self-affine fractal, which indicates that the statistical properties of surface could be the same after the certain magnifications in the horizontal and normal direction, respectively. In this case, the surface roughness under different scales could be related with the fractal dimension, D_f or Hurst exponent, H .

To make up for the deficiencies of the existing adhesion force models, this chapter proposed a set of new models for the van der Waals force and capillary force between a rough particle and a rough surface. The fractal theory and Gaussian roughness distribution were employed to resolve the problem of surface roughness. The proposed models were validated by comparing the model predictions with published experimental data. The influences of roughness, RH , contact angle and Hurst exponent towards the adhesion forces were investigated using the proposed models to explain some previously observed experimental phenomena. And the comparison between the proposed models and the existing models was also performed to explore the similarity and difference of these models.

7.2 Model development

7.2.1 Surface roughness

As suggested by previous studies [50, 212], the effective surface roughness is a crucial parameter for modeling the adhesion forces between the particles and the surface. However, the measured roughness may not necessarily be representative of the one effective to the adhesion force. A recent study of Biggerell et al. [209] showed that the surface roughness parameters increased with the scan length of measurements; that is, the measured roughness is scan length dependent. According to the fractal theory, different scan length scales taken to measure the roughness correspond to different roughness scales. The roughness of a surface under different scan length scales can be associated with [213]:

$$\sigma \approx \sigma_a (\lambda / \lambda_a)^H \quad (7.1)$$

where $H = 3 - D_f$ is the Hurst exponent defining the scaling factor, which makes the surface look the same under different magnifications. The fractal dimension, D_f , falls onto the range of 2 to 3. σ_a is the RMS roughness under the length scale λ_a , while σ is the RMS roughness under the length scale λ . λ_a is the scan size during the roughness measurement, while λ is the length seen by the particle. λ is assigned to be the nominal contact radius between the smooth particle and surface because the interaction between two contacting surfaces is inherently correlated with the contact area as investigated by the previous studies [211, 213]. Zhou et al. [50] suggested that the surface roughness within the range of the contact area should be used for the correct determination of adhesion. Ibrahim et al. [212] also found that the surface roughness “seen” by the AFM probe is related to the contact radius between the AFM probe and the surface. Based on the JKR model [54], the nominal (assumed smooth surface) contact radius $a_{JKR} = (9\pi R_p^2 \gamma / E^*)^{1/3}$, while the nominal contact radius

$a_{\text{DMT}} = (3\pi R_p^2 \gamma / 2E^*)^{1/3}$, in terms of the DMT model [55]. γ is the surface energy of adhesion and is estimated as $\gamma = \sqrt{\gamma_1 \gamma_2}$, with γ_1 and γ_2 as the surface energy of surface and particle, respectively. $E^* = [\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}]^{-1}$ is the composite Young's modulus. ν_1 and ν_2 are Poisson ratio, and E_1 and E_2 are Young's modulus for the surface and particle, respectively.

A variety of studies [65, 66, 214] have shown that the surface roughness could be represented by a Gaussian distribution of asperity height for any random rough surface:

$$p_h = \frac{1}{(2\pi)^{1/2}\sigma} e^{-h^2/(2\sigma^2)} \quad (7.2)$$

where σ is the RMS roughness under the scale λ . This would be used to represent the surface roughness feature in the following derivation.

7.2.2 Van der Waals force model

Generally, the JKR model [54] holds for large particles, high surface energies, and low elastic moduli, while the DMT model [55] is more suitable for small particles, low surface energies and high elastic moduli. Hence, both the JKR [54] and DMT models [55] would be modified to take surface roughness into consideration for the van der Waals force model. First, according to the theory of Muller et al. [215], the validity of a model in a certain set of conditions could be identified by a dimensionless parameter:

$$\mu = \frac{32}{3\pi} \left[\frac{8R_p \gamma^2}{\pi E^{*2} D^3} \right]^{1/3} \quad (7.3)$$

where $D \approx 0.3$ nm [58] is the equilibrium separation between two solids. If $\mu > 1$, the JKR model would be valid, while if $\mu < 1$, the DMT model would hold.

Based on the JKR [54] and DMT models [55], the relationships between the adhesion force for a smooth particle and surface and the contact radius are:

$$F_v = \frac{E^* a_{\text{JKR}}^3}{3R_p}. \quad (\text{JKR}) \quad (7.4)$$

$$F_v = \frac{8E^* a_{\text{DMT}}^3}{3R_p}. \quad (\text{DMT}) \quad (7.5)$$

When a non-rigid particle is in contact with a surface, the particle deforms (compression) due to the van der Waals and forms a flat contacting spot between the particle and the surface. The distance between the centre of the particle and the surface is shortened compared to a rigid particle due to this deformation. This shortened distance (or the “approach”) caused by an adhesion force can be estimated by

$$\delta_1 = \frac{1}{3R_p} \left(\frac{9\pi R_p^2 \gamma}{E^*} \right)^{2/3}. \quad (\text{JKR}) \quad (7.6)$$

$$\delta_1 = \frac{1}{R_p} \left(\frac{3\pi R_p^2 \gamma}{2E^*} \right)^{2/3}. \quad (\text{DMT}) \quad (7.7)$$

The maximum stretching of particle by the time the particle is detached from the surface can be estimated by

$$\delta_2 = \frac{1}{3R_p} \left(\frac{27\pi R_p^2 \gamma}{4E^*} \right)^{2/3}. \quad (\text{JKR}) \quad (7.8)$$

$$\delta_2 = 0. \quad (\text{DMT}) \quad (7.9)$$

The nominal (assumed smooth surface) contact area is

$$A_1 = \pi a^2. \quad (7.10)$$

Here, a represents a_{JKR} or a_{DMT} , depending on which model (either JKR or DMT model) is valid for a specific case, according to Eq. (7.3). However, for the real

contact between two rough surfaces, the effective contact area, A_2 , would be different from A_1 due to the existence of asperities such that $A_2 = CA_1$. C is the factor accounting for the percentage of actual contact area. Therefore, an effective contact radius, a' , is introduced, which is related to the nominal contact radius by

$$a' = \sqrt{C}a \quad (7.11)$$

based on Eq. (7.10). Then, this effective contact radius would be plugged into Eq. (7.4) and Eq. (7.5) to calculate the adhesion force between the rough surfaces.

Figure 7.1 A schematic diagram of the proposed van der Waals force model.

According to previous studies [73, 216], the contact between two rough surfaces could be modeled by the contact between a smooth surface and a combined rough one as shown in Figure 7.1. If the two original surfaces have the Gaussian roughness distributions, p_{h1} and p_{h2} , respectively, the combined roughness distribution for modeling could be obtained by the convolution of p_{h1} and p_{h2} as:

$$P_h(h) = \int_{-h_{\min1}}^{h_{\max1}} p_{h1}(h_1) p_{h2}(h - h_1) dh_1 = \int_{-h_{\min2}}^{h_{\max2}} p_{h1}(h_2) p_{h2}(h - h_2) dh_2 \quad (7.12)$$

where P_h is the probability of combined surface height falling between h and $h+dh$.

$h_{\min1}$, $h_{\max1}$, $h_{\min2}$ and $h_{\max2}$ are the maximum height of peak and maximum height

of valley for the two contacting surfaces (Figure 7.1). Substituting the Gaussian distribution, Eq. (7.2), into Eq. (7.12) yields (See Appendix B)

$$P_h(h) = \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} e^{-\frac{h^2}{2(\sigma_1^2 + \sigma_2^2)}}. \quad (7.13)$$

Eq. (7.6) and Eq. (7.7) give the approach between a smooth particle and surface due to adhesion, and Eq. (7.8) and Eq. (7.9) give the extension of a particle during the pull-off between a smooth particle and surface. However, for rough surfaces in contact, the approach and the stretching occur between asperities. Hence, the average radius of asperity curvature, R' , needs to be applied in Eq. (7.6) through Eq. (7.9). With the use of the method shown in Figure 7.1 where the contact between two rough surfaces was treated to be equivalent to the contact between a rough surface and a smooth one, the approach and the stretching would occur in the asperities of the rough surface touching the smooth surface. Based on the Majumdar and Bushan (MB) model, the average radius of asperity curvature can be derived as [217] (See Appendix C)

$$R' = 1.485\sigma, \quad (7.14)$$

which would be used in Eq. (7.6) through Eq. (7.9) to estimate the average approach and deformation:

$$\bar{\delta}_1 = \frac{1}{R'} \left(\frac{9\pi R'^2 \gamma}{E^*} \right)^{2/3} = 3.530 \left(\frac{\sigma^{1/2} \gamma}{E^*} \right)^{2/3}. \quad (\text{JKR}) \quad (7.15)$$

$$\bar{\delta}_1 = \frac{1}{R'} \left(\frac{3\pi R'^2 \gamma}{2E^*} \right)^{2/3} = 3.207 \left(\frac{\sigma^{1/2} \gamma}{E^*} \right)^{2/3}. \quad (\text{DMT}) \quad (7.16)$$

$$\bar{\delta}_2 = \frac{1}{3R'} \left(\frac{27\pi R'^2 \gamma}{4E^*} \right)^{2/3} = 2.914 \left(\frac{\sigma^{1/2} \gamma}{E^*} \right)^{2/3}. \quad (\text{JKR}) \quad (7.17)$$

$$\bar{\delta}_2 = 0. \quad (\text{DMT}) \quad (7.18)$$

Then, the percentage of area in contact between the particle and surface is

$$C = \int_{-h_{\min}}^{\bar{\delta}_1 + \bar{\delta}_2 - h_{\min}} P_h dh = \int_{-h_{\min}}^{\bar{\delta}_1 + \bar{\delta}_2 - h_{\min}} \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} e^{-\frac{h^2}{2(\sigma_1^2 + \sigma_2^2)}} dh =$$

$$\frac{1}{2} \left[\operatorname{erf}\left(\frac{\bar{\delta}_1 + \bar{\delta}_2 - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) - \operatorname{erf}\left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \right], \quad (7.19)$$

where $h_{\min}$ could be approximated by 2.7σ as shown during the derivation of Eq. (7.13) (See Appendix B). Similar to the derivation of Eq. (7.13), Eq. (7.19) could be approximated by

$$C = \frac{1}{2} \left[\operatorname{erf}\left(\frac{\bar{\delta}_1 + \bar{\delta}_2 - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) + 1 \right]. \quad (7.20)$$

The van der Waals force would be

$$F_V = \frac{E^* C^{3/2} a_{\text{JKR}}^3}{3R_p}. \quad (\text{JKR}) \quad (7.21)$$

$$F_V = \frac{8E^* C^{3/2} a_{\text{DMT}}^3}{3R_p}. \quad (\text{DMT}) \quad (7.22)$$

$C = 1$ as the surfaces in contact are smooth, which means that the contact area is equal to the nominal one and the adhesion force goes back to the JKR model [54] or DMT model [55] as will be shown in Figure 7.4 (a).

7.2.3 Capillary force model

A theoretical formula for the capillary force between a rough particle and surface is proposed based on the method of Butt [64]. The criterion for the formation of liquid meniscus between two objects is that the height of meniscus is at least as high as the separation between the two objects, such that the meniscus forms a bridge between them. As shown in Figure 7.2 (c), the shape of meniscus could be approximated by the toroidal geometry, which has been shown to be valid where the effect of gravity

can be neglected [218] and continuum modeling of water can be used [60] as is the case here. The toroidal geometry is prescribed by the two principal radii of curvature, r_1 and r_2 , which can be related to the Kelvin radius, r , by the Kelvin equation as

$$r = \left(\frac{1}{r_1} - \frac{1}{r_2}\right)^{-1} = -\frac{\gamma_w V_w}{R_g T' \ln(p/p_s)}, \quad (7.23)$$

where T' is the temperature, $R_g = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ is the gas constant, $V_w = 18 \times 10^{-6} \text{ m}^3/\text{mol}$ is the molar volume of water, and $\gamma_w = 0.073 \text{ N/m}$ is the surface tension of water at room temperature. p/p_s is the RH with p the vapor pressure and p_s the saturated vapor pressure. Following the same assumption of Butt [64] that the inclination of asperity surface is low, the extension of meniscus parallel to the surface would be significantly larger than that normal to the surface, which means $r_1 \ll r_2$, and $1/r_1 \gg 1/r_2$. Hence, Eq. (7.23) becomes

$$r \approx r_1 = -\frac{\gamma_w V_w}{R_g T' \ln(p/p_s)}. \quad (7.24)$$

The height of meniscus is:

$$h_l = 2cr, \quad (7.25)$$

where c is the factor related to contact angles and $c = \frac{\cos \theta_1 + \cos \theta_2}{2}$ with θ_1 and θ_2 the contact angles of surface and particle, respectively. Considering the equilibrium separation between two solids, $D \approx 0.3 \text{ nm}$ [58], the extent of height beyond D to be influenced by the meniscus is (Figure 7.2 (c)):

$$z = 2cr - D. \quad (7.26)$$

Therefore the criterion of the formation of liquid meniscus between two rough surfaces is:

$$z = 2cr - D > 0. \quad (7.27)$$

The capillary force generally has two components: the capillary pressure force and the surface tension force. However, the contribution from the surface tension force is generally small compared to the capillary pressure force, except for the case when the contact angles are approximately 90° , which rarely happens [60, 176, 219]. For simplicity, the surface tension force is ignored and the capillary force would be considered only by the capillary pressure force:

$$F_c = A\Delta P = A \frac{\gamma_w}{r} \quad (7.28)$$

where A is the area where the capillary pressure acts (covered by meniscus). $\Delta P = \frac{\gamma_w}{r}$ is the Laplace pressure. For the contact between two rough surfaces, the actual covered area (by meniscus) should be expressed by the multiplication between the maximum lateral area coverable, A_0 , (parallel to surface) and the percentage accounting for the actual covered area, $G(z)$:

$$A(z) = A_0 G(z) \quad (7.29)$$

where A_0 is equal to πR_p^2 for a spherical particle contacting with a surface (Figure 7.2 (a)). $G(z)$ would be calculated based on the surface roughness distribution as follows. Therefore, the capillary force is

$$F_c = \frac{A(z)\gamma_w}{r} = \pi R_p^2 G(z) \gamma_w / r \quad (7.30)$$

Figure 7.2 A schematic diagram of the proposed capillary force model.

The surface characteristics are treated as two parts: the apparent, nominally smooth shape (Figure 7.2 (b): (i)) and the roughness (Figure 7.2 (b): (ii)) [64]. The height distribution of the apparent nominally smooth shape is g'_h , while the surface roughness distributions of particle and surface are p_{h1} and p_{h2} , respectively. P_h , Eq. (7.13), is the convolution of the surface roughness distributions of particle and surface, p_{h1} and p_{h2} (Eq. (7.12)) as shown in the van der Waals force model. The overall height distribution is resultant by

$$g_h(z) = \int_0^{H_{\max}} g'_h(\zeta) P_h(\zeta - z) d\zeta \quad (7.31)$$

where $H_{\max}$ is the maximum separation distance available for the formation of meniscus and is equal to R_p for the contact between a spherical particle and a surface. The deformation of particle is neglected here for the capillary force calculation, since it is far smaller than $H_{\max}$. Therefore, the percentage of area covered by the meniscus is calculated by the integration of $g_h(z)$ from $-h_{\min}$ to $z - h_{\min}$:

$$G(z) = \int_{-h_{\min}}^{z-h_{\min}} g_h(\zeta) d\zeta \quad (7.32)$$

where $h_{\min} = h_{\min1} + h_{\min2}$.

Based on the joint probability distribution of surface roughness, Eq. (7.13), and the height distribution of the apparent nominally smooth shape, $g'_h = \frac{2}{R_p^2} (R_p - z)$ [64], the percentage of area covered by the meniscus, $G(z)$, can finally be derived as (See Appendix D)

$$\begin{aligned} G(z) = & \frac{1}{R_p} \left\{ z - \right. \\ & \left[(z - h_{\min}) \operatorname{erf} \left(-\frac{z-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \right. \\ & \left. \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(z-h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} - (-h_{\min}) \operatorname{erf} \left(\frac{h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) + \right. \\ & \left. \left. \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} \right] \right\} - \frac{\sigma_1^2 + \sigma_2^2}{R_p^2} \left[\operatorname{erf} \left(\frac{z-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \right. \end{aligned} \quad (7.33)$$

$$\left. \operatorname{erf}\left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \right].$$

The solution consists of six terms with the last term having two error functions. The first term represents the RH effect. The second, third and last terms represent the coupling effect of RH with surface roughness, while the fourth and fifth terms represent the roughness effect solely. A careful inspection of each term in Eq. (7.33) would show that the last term should generally be several orders of magnitude smaller than the other terms, since $\sqrt{\sigma_1^2 + \sigma_2^2}/R_p \ll 1$ would generally hold. This has been further confirmed by the more detailed analysis of comparing the absolute value of these separate terms versus the surface roughness and the RH (See Appendix E). Despite being negligible for the case $\sqrt{\sigma_1^2 + \sigma_2^2}/R_p \ll 1$, this term would not be neglected in the calculation of this work. Consequently, the area covered by the meniscus is

$$\begin{aligned}
A(z) = \pi R_p \left\{ z - \left[(z - h_{\min}) \operatorname{erf}\left(-\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \right. \right. \\
- \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(z - h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} \\
- (-h_{\min}) \operatorname{erf}\left(\frac{h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \\
\left. \left. + \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} \right] \right\} \\
- \pi(\sigma_1^2 + \sigma_2^2) \left[\operatorname{erf}\left(\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) - \operatorname{erf}\left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \right].
\end{aligned} \tag{7.34}$$

And the capillary force is

$$\begin{aligned}
 F_c = \frac{A(z)\gamma_w}{r} = \frac{\pi R_p \gamma_w}{r} & \left\{ z - \left[(z - h_{\min}) \operatorname{erf} \left(-\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \right. \right. \\
 & \left. \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(z - h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} - \right. \\
 & \left. (-h_{\min}) \operatorname{erf} \left(\frac{h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) + \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} \right] \right\} - \\
 & \frac{\pi(\sigma_1^2 + \sigma_2^2)\gamma_w}{r} \left[\operatorname{erf} \left(\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \operatorname{erf} \left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) \right].
 \end{aligned} \tag{7.35}$$

For a smooth particle on a smooth surface, $h_{\min} = 0$, $K = 0$ and $\operatorname{erf} \left(-\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) = -1$, which leads to $G(z) = \frac{2z}{R_p} = \frac{2(2cr - D)}{R_p}$. Correspondingly, the capillary force, Eq. (7.35), devolves to

$$F_c = \frac{\pi R_p^2 G(z) \gamma_w}{r} = \frac{2\pi R_p (2cr - D) \gamma_w}{r}. \tag{7.36}$$

This is consistent with the models of Derjaguin [220] and Butt [64] for the contact between smooth surfaces. When $2cr \gg D$, the equilibrium separation distance D could be assumed to be zero and Eq. (7.36) could be further simplified to

$$F_c = 4\pi R_p c \gamma_w = 2\pi R_p (\cos\theta_1 + \cos\theta_2) \gamma_w. \tag{7.37}$$

This is the same as the derived classical models for a smooth particle on a smooth surface by Orr et al. [59], Pakarnen et al. [60] which predict the capillary force to be independent of RH.

Finally, the total adhesion force is

$$F_A = F_v + F_c. \quad (7.38)$$

It should be noted that the currently proposed capillary force model is applicable for the capillary phenomenon of volatile liquid (e.g., water). Hence, in order to predict the adhesion force, including the capillary force from non-volatile liquid as measured by Rabinovich et al. [221], a further modification to the proposed model should be needed. However, it is beyond the scope of the current work and left as a task for future study.

The proposed model considers elastic deformation only, but partial or full plastic deformation may occur when the resultant stress from the adhesion force between a particle and a surface exceeds the yield strength of the material(s) involved. The understanding about the effect of plastic deformation in particle-surface adhesion force is far from complete, both experimentally and theoretically. There is still some controversy about the onset of plastic deformation from the experiments. For example, Zhou and Peukert [222] found that a 10 μm polystyrene particle could be plastically deformed when it contacted with a rough surface. A similar conclusion about a 5 μm polystyrene particle on an atomically smooth mica surface was reached in the study of Biggs and Spinks [223]. Contrarily, Cleaver and Looi [224] found that there was almost no plastic deformation for the contact between 12 μm polystyrene particles, if no external force was added to the contact. The study of Heim et al. [225] showed that the effect of plastic deformation in the adhesion force could be negligible between the contact of 2~20 μm polystyrene and gold particles, even when an external load up to 1 μN was added to the contact.

Existing models [226, 227] do not fully account for the effect of plastic deformation in adhesion force for the contact between a smooth particle and surface. The theoretical consideration of the effect of plastic deformation in the adhesion force between a rough particle and surface could be more complex and beyond the scope of this work. However, previous studies [222, 223, 228] showed that the impact on adhesion force due to the adhesion force-induced plastic deformation compared to the sole elastic deformation were no more than a factor of 2. Neglecting the plastic deformation in the proposed model should not impose major error to the model predictions. In the following model validation part, the experimental data from the studies where no plastic deformation was explicitly mentioned or observed were intentionally selected, which might further reduce the possible prediction error due to the neglecting of plastic deformation.

7.3 Model validation

The predictions from the proposed models were compared against the experimental data from Beach et al. [208] (Ref. 1), Segeren et al. [229] (Ref. 2), Paajanen et al. [230] (Ref. 3), Zwol et al. [231] (Ref. 4), Ata et al. [232] (Ref. 5), Matope et al. [233] (Ref. 6), Rabinovich et al. [57] (Ref. 7), Rabinovich et al. [63] (Ref. 8), Jacobs et al. [234] (Ref. 9), Leite et al. [235] (Ref. 10), Tormoen et al. [236] (Ref. 11), Fukunish and Mori [237] (Ref. 12), and Sedin and Rowlen [238] (Ref. 13). The study of Beach et al. [208] measured the adhesion force between glass (Gl) and polystyrene (PS) particles and the polypropylene (PP) surface with atomic force microscope (AFM). The Hamaker constants of particles and surface needed for model predictions were

taken from the study of Beach et al. [208] together with the relationship between the Hamaker constant and surface energy:

$$A_h = 1.44 \times 10^{-18} \gamma. \quad (7.39)$$

The exact value of RH has not been given in the study [208], instead it was denoted that the RH was no more than 30%. In the validation, the RH of 30% was used. Two scan sizes, $\lambda_{a1} = 20$ and $\lambda_{a2} = 5$ μm , were used during the surface roughness measurements in the study [208], which resulted in several sets of σ_{a1} and σ_{a2} . They are plugged into Eq. (7.1) to estimate the Hurst exponent (calculated $H = 0.93$). However, for other experimental studies, only one scan size was used which makes the calculation of H impossible. Considering the Hurst exponent of 0.93 from the study of Beach et al. [208] and the typical value of the Hurst exponent is around 0.8 [213], $H = 0.9$ is used in Eq. (7.1) for the rest of the cases. Actually, the selection of this value would bring little influence to the predictions as to be shown below. The roughness of particle was not given in the study of Beach et al. [208], which is assumed negligible compared to the roughness of surface. The study of Segeren et al. [229] measured the adhesion force between silica (Sil) particles and silicon (Si) surfaces of different roughness levels. Paajanen et al. [230] measured the adhesion force between silica (Sil) spheres and silica (Sil) surface with respect to the RH from 0% to 80%. The roughness of particle is assumed to be negligible as well for this study. The adhesion force between borosilicate glass (Gl) spheres and gold-coated polystyrene (G-PS) particles and gold (Gd) surfaces have been measured by Zwol et al. [231], under the RH of 40%. The roughness provided there was the combined particle and surface roughness, as listed in Table 7.1. The scan size has not been given and 10 μm is assumed. The study of Ata et al. [232] measured the adhesion force between a glass (Gl) sphere and silver (Ag) and alumina (AlO) substrates as a

function of RH. The study of Matope et al. [233] presented the adhesion forces between a silica (Sil) sphere and three types of metallic film surface [silver (Ag), copper (Cu), and aluminum (Al)] with the roughness ranging from 0.5 to 3 nm. Rabinovich et al. [57] measured the adhesion force between a glass (Gl) sphere and titanium (Ti) film surface. The RMS roughness of particle was mentioned to be less than 0.2 nm in the study [57], and 0.15 nm is assumed for the model predictions. The scan length is assumed to be 5 and 20 μm for the particle and surface, respectively. The study of Rabinovich et al. [63] measured the adhesion forces between a glass sphere and various types of substrates [silicon (Si), silica (Sil), sapphire (Sa), titanium (Ti) and silver (Ag)], as a function of RH. A particle RMS roughness of 0.15 nm is also assumed for the model predictions. Jacobs et al. [234] measured the adhesion forces between diamond (D) surface and diamond-like carbon (DLC) and ultrananocrystalline diamond (UNCD)-coated silicon AFM tip of the radii ranged from 2.33 to 115.51 nm. The scan size for measuring roughness of the tip was not given but was suggested to be related to the radius of the tip. Hence, the assumed scan sizes as listed in Table 7.1 would be applied for the model predictions. Although the RH during the experiments was not given, no capillary force related phenomenon was mentioned in the study. Hence, it is assumed that the RH was low (10%) here. The study of Leite et al. [235] showed the adhesion force between the mica (Mic) surface and oxidized silicon (O-Si) AFM tip. Tormoen et al. [236] measured the adhesion force between gold-coated (Gd) wafer and gold-coated (Gd) silicon AFM tips modified with self-assembled monolayers (SAM). Fukunishi and Mori [237] measured the adhesion forces between the glass (Gl-W) particle washed by a mixed solution and surfaces of mica (Mic) and silica (Si-W) washed by a mixed solution under different RHs. They also measured the adhesion forces between a silicon (Si)

AFM tip and surfaces of silica (Sil-W) washed by a mixed solution and of etched silica (Sil-E) under different RHs. The study of Sedin and Rowlen [238] presented the adhesion force between the silica-terminated AFM tip and mica (Mic) surface, as a function of RH. The relevant parameters for the model predictions of all these studies are listed in Table 7.1.

The process of calculating the total adhesion force is as follows:

- (1) The dimensionless parameter, μ (Eq. (7.3)), is calculated to determine which van der Waals force model (JKR-based or DMT-based) is valid for the van der Waals force prediction for a given case. According to the calculation, $\mu > 1$ is obtained for most of experimental cases and thus the JKR-based model is valid for these cases, while the DMT-based model holds for some cases (highlighted in Figure 7.3) from the studies of Jacobs et al. [234], Leite et al. [235], Tormoen et al. [236], and Sedin and Rowlen [238] where the particles or tips of nano-sized radii and surfaces (e.g., diamond) of high moduli were applied.
- (2) The van der Waals force, Eq. (7.21) or Eq. (7.22), is calculated and then the criterion of capillary condensation, Eq. (7.27), is checked.
- (3) If the criterion is not satisfied, indicating no capillary force is induced, the van der Waals force will serve as the total adhesion force.
- (4) Otherwise, the capillary force, Eq. (7.35), is subsequently calculated and added to the van der Waals force to result in the total adhesion force, Eq. (7.38).

The comparison between the predictions of models and the experimental data is shown in Figure 7.3.

Table 7.1 Parameters for the model predictions against the existing experimental data.

Reference	Surface/ Particle	R_p (μm)	$\gamma_1 \cdot (\text{J}/\text{m}^2) / \gamma_2$ (J/m^2)	θ_1/θ_2	RH (%)	σ_1 (nm)/ λ_{a1} (μm)	σ_2 (nm)/ λ_{a2} (μm)	H	E_1/E_2 (GPa)	v_1/v_2
Ref. 1	PP/GI	4.76	0.034/0.04	109° /30°	30	6.53- 39.58/5	0	0.93	0.8/69	0.42/0. 22
Ref. 1	PP/PS	4.07	0.034/0.046	95° /66°	30	6.53- 39.58/5	0	0.93	0.8/1	0.42/0. 35
Ref. 2	Si/Sil	2.5	0.09/0.09	50° /70°	40	0.1- 17.27/10	0.18/0.3 5	0.90	130/100	0.25/0. 25
Ref. 3	Sil/Sil	1.0, 2.5	0.09/0.09	70°/70 °	0- 80	0.141/1	0	0.90	100/100	0.25/0. 25
Ref. 4	Gd/GI	17.3	0.28/0.04	70° /30°	40	1.79-7.73/10		0.90	78/69	0.42/0. 22
Ref. 4	Gd/G-PS	99.5	0.28/0.046	70°/70 °	40	2.59-8.81/10		0.90	78/1	0.42/0. 35
Ref. 5	Ag/GI	10	0.28/0.04	60° /30°	18- 70	1.2/20	0.2/5	0.90	85/69	0.37/0. 22
Ref. 5	AlO/GI	10	0.17/0.04	100° /30°	0- 80	0.2/20	0.2/5	0.90	37/69	0.23/0. 22
Ref. 6	Ag/Sil	2.5	0.28/0.09	60° /70°	20	0.5- 1.41/10	0.2/1	0.90	85/100	0.37/0. 25
Ref. 6	Cu/Sil	2.5	0.14/0.09	60° /70°	20	0.9- 2.72/10	0.2/1	0.90	68/100	0.34/0. 25
Ref. 6	Al/Sil	2.5	0.17/0.09	90° /70°	20	1.2, 2.3/10	0.2/1	0.90	75.9/10 0	0.33/0. 25
Ref. 7	Ti/GI	10	0.21/0.04	100° /30°	25	0.17, 1.64/20	0.15/5	0.90	120/69	0.26/0. 22
Ref. 8	O-Si/GI	30	0.09/0.04	50° /30°	0- 77	0.2/30	0.15/15	0.90	130/69	0.25/0. 22
Ref. 8	P-Sil/GI	30	0.09/0.04	60° /30°	0- 72	0.3/30	0.15/15	0.90	100/69	0.25/0. 22
Ref. 8	E-Sil/GI	30	0.09/0.04	105° /30°	42- 80	0.7/30	0.15/15	0.90	100/69	0.25/0. 22
Ref. 8	Sa/GI	30	0.17/0.04	95° /30°	0- 67	0.3/30	0.15/15	0.90	37/69	0.23/0. 22
Ref. 8	Ti/GI	30	0.21/0.04	100° /30°	25- 76	1.4/30	0.15/15	0.90	120/69	0.26/0. 22
Ref. 8	Ag/GI	30	0.28/0.09	60° /30°	28- 70	3/30	0.15/15	0.90	85/69	0.37/0. 22
Ref. 9	D/DLC-Si	0.0023 3- 0.0174 0.0025	0.21/0.49	60° /60°	10	0.091/0. 1	0.033- 0.548/0. 005-0.1	0.90	1000/13 0	0.06/0. 25
Ref. 9	D/UNCD-Si	6- 0.1155 1	0.21/0.7	60° /60°	10	0.091/0. 1	0.031- 1.576/0. 005-0.45	0.90	1000/13 0	0.06/0. 25

Ref. 10	Mic/O-Si	0.023	0.07/0.09	0°/79°	47	0.1/1	0	0.90	171/130	0.3/0.2 5
Ref. 11	Gd/Gd-Si	0.053, 0.032	0.28/0.028- 0.055	70° /29°- 51°	10	1/2	0	0.90	78/130	0.42/0. 25
Ref. 12	Mic/Gl-W	8	0.07/0.347	0°/35°	8- 80	0.05/20	0.13/2	0.90	171/69	0.3/0.2 2
Ref. 12	Sil-W/Gl- W	8	0.125/0.347	45°/35°	8- 80	0.1/20	0.13/2	0.90	100/69	0.25/0. 22
Ref. 12	Sil-W/Si	0.09	0.125/0.09	45°/50°	8- 80	0.1/20	0	0.90	100/130	0.25/0. 25
Ref. 12	Sil-E/Si	0.09	0.125/0.09	51°/50°	8- 80	0.18/20	0	0.90	100/130	0.25/0. 25
Ref. 13	Mic/Sil	0.01	0.07/0.09	0°/70°	0- 74	0.03/1	0	0.90	171/100	0.3/0.2 5

*: The subscripts 1 and 2 denote surface and particle, respectively.

It is shown in Figure 7.3 that the model predictions are in a good agreement with the experimental data and the difference between the model predictions and the experimental data generally falls within 1 order of magnitude, which validates the derived models of van der Waals force and capillary force. The proposed models employ the fractal theory to correlate the surface RMS roughnesses under different scan lengths (sizes) and regard that the *effective* RMS roughness corresponding to the nominal contact radius determines the adhesion forces. The proposed models use the *effective* RMS roughness converted (Eq. (7.1)) from the *actual* (or measured) RMS roughness, making the proposed model applicable to a wide range of *actual* RMS roughness (from nano- to milliscale). Figure 7.3 shows that the model predictions are reasonably close to the experimental data, corresponding to the RMS roughness of about 0.4 μm under the scan length of 20 μm from the study of Beach et al. [208] (Ref. 1).

Figure 7.3 The comparison between the predictions of the proposed models and the experimental data. The red dash lines specify 1 order of magnitude difference between the model predictions and experimental data, while the black line indicates the perfect match between the model predictions and the experimental data.

7.4 Parameter investigation

The proposed models enable the prediction of van der Waals force and capillary force between a rough particle and surface free of the limitation of roughness scales compared to the existing models commonly valid for nanoscale roughness. The capillary force model also captures the effect of RH on capillary force, which is important for relating the environmental humidity to the adhesion force. These would contribute to expand the capability of the adhesion force relevant analysis. As follows, a variety of associated parameters, including surface roughness, RH, contact angle and Hurst exponent, would be investigated. The parameter investigation was based on

the case of 2.5 μm silica particle on the silica surface from the study of Paajanen et al. [230] by varying the very parameter.

The attempt is made to compare the proposed models of this work with the existing models, including the van der Waals force model of Rabinovich et al. [57] (Eq. (2.1)), the capillary force model of Rabinovich et al. [63] (Eq. (2.2)), and the capillary force model of Butt [64] (Eq. (2.3)). The equilibrium distance, $D \approx 0.3 \text{ nm}$ was used for the capillary force model of Rabinovich et al. [63]. The roughness parameter, δ_0 in the model of Butt [64], is approximated by $2h_{\min} = 5.4\sigma$ for the comparison.

7.4.1 Surface roughness

Surface roughness influences the van der Waals force and the capillary force by affecting the contact area and the capillary condensation between a particle and a surface, respectively. Schaefer et al. [239] found that the measured adhesion force between the rough surfaces could be a factor of 50 smaller than the theoretical value for the smooth surfaces from the JKR model. Coelho and Harnby [240] indicated that surface roughness significantly affected the capillary adhesion force by decreasing the effective adsorbed layer thickness. Zwol [231] mentioned that the capillary force is so sensitive to nanoscale roughness that the increase of RMS roughness from 2.5 – 6 nm could lead to a 2 orders of magnitude decrease of capillary force.

As mentioned during the model derivation, the measured RMS roughness generally corresponds to a certain scan length; that is, the measured RMS roughness is scan length (size) dependent. If there are two surfaces measured to have the same RMS

roughness under different scan lengths, the surface under the smaller scan length should be rougher than another one. The effect of the same roughness under different scan lengths on the adhesion forces should be different, which has been considered by the proposed models of this work. Hence, for the illustrative purpose, two scan lengths (0.1 and 1 μm) for the same roughness range (0 – 5 nm) are employed for the following parameter investigation based on the models of this work. A RMS roughness range of 0 – 5 nm was used to represent the smooth (0 nm) to extremely rough (5 nm) surface in the parameter investigation. According to existing studies [229, 241], it was regarded that 10 nm of RMS roughness under the scan length of 10 μm was extremely rough. In the current study, 0.1 μm and 1 μm scan lengths are used. Using Eq. (7.1), 5 nm of RMS surface roughness under 0.1 μm and 1 μm scan lengths corresponds to an RMS surface roughness way larger than 10 nm under a 10 μm scan length. In the current model predictions, when the RMS roughness goes above 5 nm, the adhesion forces are not sensitive to the change in roughness. The RH is set to be 40%, and the values of all other parameters are the same as those shown in Table 7.1. The results are shown by Figure 7.4 (a) and the predictions by the classical van der Waals force [54] and capillary force models [64] for the contact between a smooth particle and surface are also added for the illustrative purposes.

The predictions from the existing models are also added to Figure 7.4 (a) for comparison. The peak-to-peak distance is needed for the model prediction of Rabinovich et al. [57]. However, the peak-to-peak distance cannot be determined with only knowledge of the RMS roughness. Hence, a simplified operation is performed: the peak-to-peak distance for every RMS roughness is calculated by multiplying the roughness with 280 which is the multiplier between the peak-to-peak distance and

RMS roughness in the basic case from Segeren et al. [229]. The variation of adhesion forces within the roughness range of 0 – 0.15 nm is redrawn as Figure 7.4 (b) to better show the model comparison within the small RMS roughness range.

Figure 7.4 The influence of roughness towards the van der Waals force and capillary force based on the models of this work and the existing studies for (a) RMS roughness range from 0 – 5 nm and (b) RMS roughness range from 0 – 0.15 nm. The constant parameters for modeling are listed in Table 7.1.

It is shown by the models of this work that the decrease of the adhesion forces could be several orders of magnitude, when the RMS roughness increases from 0 to 5 nm. The decreasing trend generally follows the pattern that it is very fast initially and then gradually becomes slower. Rabinovich et al [57] experimentally observed the same trend with the AFM measurements. Cheng et al. [242] also presented a similar pattern with their numerical calculations of van der Waals force. Also shown are the predictions from the classical solutions of the van der Waals force (JKR model [54]) and capillary force [64] between a smooth particle and surface. When the surface

roughness is asymptotic to zero, the predictions from the models of this work converge to the classical solutions. For the contact between a smooth particle and surface, the van der Waals force (Eq. (7.4)) is about 10 times larger than the capillary force (Eq. (7.36)). This is because (1) the surface energy used for van der Waals force calculation is moderately large (0.09 J/m^2) and (2) the RH is not high (40%) and the contact angle is large (e.g., 70°) for the contact. If the situation is reversed, that is, the surface energy is small, while the RH is high (e.g., 80%) and the contact angle is small (e.g., 20°), the capillary force could be significantly larger than the van der Waals force for the smooth contact.

It is shown that the model of Rabinovich et al. [63] predicts a quick decrease of capillary force from 200 to 0 nN, as the roughness increases from 0 to 0.056 nm, which should be related to the mandatory applicability condition of this model: $(H_c + D) \leq 2rc$ (where H_c is the separation between a particle and the average surface plane caused by an asperity). This condition enforces the capillary force to be zero once the equals sign is satisfied, whatever the actual capillary force. It is also shown that the existing models do not consider that the RMS roughness is scan size dependent. Hence, these models will provide different adhesion results for the same particle-surface contact with the different RMS roughness data under the different scan lengths, which should be unreasonable.

7.4.2 RH

Several previous experimental studies [61, 62, 243] showed that the adhesion force between hydrophilic surfaces increases acutely as the RH increases. For instance, the

adhesion force could be increased by a factor of 2 – 5 all the way from 5% to 90% depending on various parameters such as particle size and surface roughness [243]. Çolak et al. [62] observed that the increase of adhesion force with RH was sharper at the range of 30% to 70%. In order to investigate the effect of RH in the adhesion forces, the RH is varied from 5% to 95%. The predictions from the existing models are also added for comparison. The adhesion forces are predicted by the models of this work under two different scan lengths (0.1 and 1 μm) for the same roughness (0.141 nm). The values of all other parameters are the same as those shown in Table 7.1. The results are shown by Figure 7.5.

Figure 7.5 The influence of RH towards the van der Waals force and capillary force based on the models of this work and the existing studies. The constant parameters for modeling are listed in Table 7.1.

It is shown by the model of this work that the variation of capillary force with respect to RH follows the pattern: when $\text{RH} < 30\%$ (critical RH), the capillary force is 0 as

the criterion of meniscus formation (Eq. (7.27)) is not satisfied; when $RH > 30\%$, the capillary force is formed and increases as the RH. This pattern of capillary force variation has also been observed in the previous experiments [63, 230] and is consistent with the description about liquid meniscus formation by Coelho and Harnby [244]. When $RH > 30\%$, the capillary force for the scan length of $1\ \mu\text{m}$ is always larger than that for the scan length of $0.1\ \mu\text{m}$. This is because the scan length of $1\ \mu\text{m}$ corresponds to a smoother surface for the same RMS roughness than the scan length of $0.1\ \mu\text{m}$, and thus more liquid condensation could be formed between the particle and surface under the same RH.

The capillary force model of this work and that developed by Butt [64] predict the same critical RH (30%) due to the same criterion of meniscus formation used. However, the model developed by Rabinovich et al. [63] predicts a higher critical RH (52%). This is because the critical RH is determined by the condition $(H_c + D) = 2rc$ in the model by Rabinovich et al. [63], which leads to a larger RH compared to the criterion of the current model as well as Butt's model [64], Eq. (7.27). Additionally, it is shown that both the proposed model of this work and the model of Rabinovich et al. [57] predict a constant van der Waals force with respect to RH. However, it should be noted that van der Waals force may decrease with increasing RH, since the condensed meniscus at the interface between a particle and a surface could lead to the decrease of Hamaker constant (surface energy) and thus the van der Waals force. Rabinovich et al. [63] developed an approximate method to account for the effect of meniscus in Hamaker constant for a contact between a *smooth* particle and surface. However, it will be more difficult to account the effect of meniscus in Hamaker constant for a *rough* contact. The framework of the proposed model allows for the incorporation of

the humidity effect on the Hamaker constant, but instead of using the Hamaker constant, an *effective* Hamaker constant (surface energy), as suggested by Kim et al. [245], should be used. At present, the knowledge about the variation of the *effective* Hamaker constant with respect to RH is still rare. The humidity effect on van der Waal force is not included in the currently proposed model. Another reason is that when the Hamaker constant is significantly affected by the condensed liquid, there should be a significant amount of liquid condensed between a particle and a surface, which might suggest the dominance of capillary force over the van der Waals force (e.g., RH>60% as shown by the predictions from the models of this work in Figure 7.5). Therefore, the variation of van der Waals force in this case should have a minor effect on the total adhesion force, which is the summation of capillary force and van der Waals force.

7.4.3 Contact angle

The contact angle has been generally used to describe the relative hydrophobicity and hydrophilicity of a surface and is related to the formation of the meniscus between a particle and a surface, and thus the capillary force. The study of Hsiao et al. [246] showed that the capillary force decreased as the contact angle increased from 0° to 90° and attributed this to the decrease of meniscus size. The decreasing trend of adhesion force versus contact angle was also found by De Souza et al. [247] for two parallel flat plates. In order to investigate the effect of contact angle in the adhesion force, the particle and surface are set to have the same contact angle varied from 5° to 95° under the RH of 40%. The adhesion forces are predicted by the models of this work under two different scan lengths (0.1 and 1 μm) for the same roughness (0.141 nm). The

predictions from the existing models are added for comparison. The values of all other parameters are the same as those shown in Table 7.1. The results are shown by Figure 7.6.

Figure 7.6 The influence of contact angle towards the van der Waals force and capillary force based on the models of this work and the existing studies. The constant parameters for modeling are listed in Table 7.1.

The capillary force model of this work predicts that the capillary force disappears due to the incapability of forming the meniscus between the particle and surface under the RH of 40%, when the contact angle is larger than 75°. That is, for a given level of RH, there is a critical contact angle above which the capillary force would not exist. Consequently, similar to the case of RH, a two-stage pattern for the capillary force variation as the contact angle is also predicted. The model of this work predicts that the capillary force for the scan length of 1 μm is always larger than that for the scan

length of 0.1 μm , which is due to the fact that the scan length of 1 μm corresponds to the smoother surface for the same roughness.

The critical contact angle predicted by the current model is the same as the one predicted by the model developed by Butt [64]. However, this critical contact angle is larger than the one predicted by the model of Rabinovich et al. [63]. It is due to the fact that the critical contact angle is determined by the condition $(H_c + D) = 2rc$ in the model by Rabinovich et al. [63] compared to $D = 2rc$ in the current model and Butt's model.

7.4.4 Hurst exponent

Based on the fractal theory, the Hurst exponent is used for calculating the surface roughness effective for the adhesion forces in the proposed models. This exponent is related to the fractal dimension, D_f , by $H = 3 - D_f$ with $2 < D_f < 3$ that makes $0 < H < 1$. For the same type of surface, the rougher surfaces will have the higher fractal dimension [248]. The relationship between the adhesion force and the fractal dimension (Hurst exponent) has rarely been explored. Until recently, the study of Tanaka et al. [249] experimentally showed that the adhesion force between two toner particles was inversely proportional to the fractal dimension and thus proportional to the Hurst exponent. The influence of the Hurst exponent towards the adhesion forces is shown in Figure 7.7 with the Hurst exponent varied from 0.05 to 0.95 under the RH of 40%. Since the concrete relationship between the surface roughness and the Hurst exponent is impossible to define, the RMS roughness is fixed to be 0.141 nm. The adhesion forces are predicted by the models of this work under two different scan

lengths (0.1 and 1 μm) for the same roughness. The values of all other parameters are the same as those shown in Table 7.1.

Figure 7.7 The influence of Hurst exponent towards the van der Waals force and capillary force based on the models of this work. The constant parameters for modeling are listed in Table 7.1.

Figure 7.7 shows that the adhesion forces generally increase as the Hurst exponent, which is consistent with the existing experimental results [249]. Considering that the typical value of Hurst exponent is 0.8 and the reported values of Hurst exponent for various surfaces are mainly distributed in the range of 0.6 to 1 [250-253], the error produced by using 0.9 falls on average within a factor of 2 and 3 for the scan lengths of 0.1 and 1 μm , respectively, which further justifies the use of the Hurst exponent equal to 0.9 during the model validation. But the actual value of the Hurst exponent or fractal dimension would be preferred whenever it is available from the measurements or literatures.

7.5 Conclusions

The understanding of the adhesion forces between a rough particle and surface is of practical significance for modeling particle resuspension processes. Previously proposed models are subject to various limitations in predicting the van der Waals force and capillary force between a rough particle and surface. Aiming to overcome these limitations, a set of new mathematical models for the van der Waals force and capillary force between a rough particle and surface is developed, by considering the characteristic of multiple roughness scales with the fractal theory and the Gaussian distribution of surface roughness. The new models are validated against the existing experimental data, showing good agreement. The new models converge to the classical solutions for the contact between a smooth particle and surface.

With the use of the new models, the influences of roughness for the combination of particle and surface, RH, contact angle and Hurst exponent towards the particle-surface adhesion forces have been investigated. The decline mode of the adhesion force with surface roughness and contact angle as well as the increase mode with RH and Hurst exponent observed previously can now be reasonably explained by the new models. And the comparison between the models of this work and the existing studies has also been performed during the parameter investigations in terms of roughness, RH, and contact angle. The models of this work identify the fact that the RMS roughness is scan length dependent and thus consider the effect of roughness together with the corresponding scan length based on the fractal theory compared to the existing models.

The new models contribute to calculate the mean van der Waals force and capillary force, whereas the adhesion force between particles and the surface generally follows

a distribution (e.g., log-normal distribution and Weibull distribution) in reality. Hence, the sole mean adhesion force does not fully account for the adhesion force distribution between rough particles and the surface. In next chapter, the concept of adhesion force distribution would be introduced and a more complete picture about the adhesion force distribution between rough particles and the surface would be developed based on the relevant centrifuge experiments.

Chapter 8 Development of Adhesion Force Distribution Model

8.1 Introduction

The developed models in Chapter 7 related the adhesion forces with the RMS roughness. If a surface is divided into some sub-areas, it is possible that the surface morphology and, thus, the RMS roughness will vary from sub-area to sub-area. In other words, there will be a distribution of RMS roughness in terms of location. When identical particles are deposited onto different sub-areas of a surface, different RMS roughnesses may be experienced by these particles, which will lead to the adhesion force of different magnitudes, and thus an adhesion force distribution according to the models of Chapter 7. Ideally, if identical smooth particles contact with a smooth surface, there will be no distribution, because of the same RMS roughness (i.e., zero) everywhere. Actually, existing studies [50, 68, 254, 255] have suggested that the distribution of adhesion force should be resultant from the distribution of surface roughness. If the RMS roughness distribution could be figured out, integrating the RMS roughness distribution into the mean adhesion force models could lead to the development of an adhesion force distribution model. It should be noted that the RMS roughness distribution is different from the Gaussian roughness distribution of asperity height (Eq. (7.2)) described in Chapter 7.

In this chapter, a general adhesion force distribution model was developed by integrating the RMS roughness distribution into the mean adhesion force models of Chapter 7. The integration was performed by both a statistical analysis method and

Monte Carlo simulation. In order to validate the proposed model, the measured adhesion force distributions from a series of centrifuge experiments were compared with model predictions. Further validation was accomplished by comparing model predictions with existing experimental data. Finally, the effect of RMS roughness distribution on the adhesion force distribution was explored based on the proposed model.

8.2 Adhesion force distribution model

The morphology of a surface varies from sub-area to sub-area. Correspondingly, the RMS roughnesses may be different for different sub-areas [68]. In other words, the RMS roughnesses for different locations of a surface may follow a certain distribution. When particles are deposited onto different sub-areas of a surface (Figure 8.1), the resultant RMS roughness $\sigma = \sqrt{(\sigma_1^2 + \sigma_2^2)}$ for different particles could be different due to the existence of a RMS roughness distribution. As a result, this will lead to the variation of adhesion force from particle to particle according to the mean adhesion force models (Eq. (7.21) or Eq. (7.22) for van der Waals force and Eq. (7.35) for capillary force), that is, the distribution of adhesion force. Once the RMS roughness distribution is known, the adhesion force distribution model could be developed by integrating the RMS roughness distribution into the mean adhesion force models (Eq. (7.21) or Eq. (7.22) and Eq. (7.35)), via either a statistical analysis method or Monte Carlo simulation. The mean adhesion force models of Chapter 7 are not repeated. The methods (statistical analysis and Monte Carlo simulation) that are used to integrate the RMS roughness distribution into the mean adhesion force models are presented as follows.

Figure 8.1 A schematic diagram of adhesion force distribution model.

8.2.1 Statistical analysis

Let Σ_1 and Σ_2 be the random variables representing the RMS roughness on the surface and particle, respectively, and the probability density distributions for Σ_1 and Σ_2 are $f_{\Sigma_1}(\sigma_1)$ and $f_{\Sigma_2}(\sigma_2)$, respectively. Let X_1 and X_2 be the independent random variables representing the mean square roughnesses on the surface and particle, respectively; that is, $X_1 = \Sigma_1^2$ and $X_2 = \Sigma_2^2$. If $f_{\Sigma_1}(\sigma_1)$ and $f_{\Sigma_2}(\sigma_2)$ are continuous probability distribution, the corresponding distributions for X_1 and X_2 will be

$$\begin{aligned} f_{X_1}(x_1) &= f_1(\sqrt{x_1})/2\sqrt{x_1} \text{ and} \\ f_{X_2}(x_2) &= f_1(\sqrt{x_2})/2\sqrt{x_2}, \end{aligned} \quad (8.1)$$

respectively. Then, the distribution of random variable $Y = X_1 + X_2$ is obtained by the convolution of $f_{X_1}(x_1)$ and $f_{X_2}(x_2)$ as:

$$f_Y(y_r) = \int_{x_{1\min}}^{x_{1\max}} f_{X_1}(x_1) f_{X_2}(y_r - x_1) dx_1 = \int_{x_{2\min}}^{x_{2\max}} f_{X_1}(x_2) f_{X_2}(y_r - x_2) dx_2, \quad (8.2)$$

where Y actually accounts for the sum of the mean square roughnesses for the surface and particle; that is, $Y = \Sigma_1^2 + \Sigma_2^2$.

According to Eq. (7.21), Eq. (7.22) and Eq. (7.35), the adhesion force is a decreasing function of Y , ($f' = u_f(y_r)$), which has the inverse function of $y_r = v_f(f')$. Hence, the cumulative probability distribution of adhesion force F' is

$$\begin{aligned} J_{F'}(f') &= P(F' \leq f') = P(u_f(y_r) \leq f') = P(y_r \geq \\ v_f(f')) &= 1 - P(y_r \leq v_f(f')) = 1 - \int_{y_{\min}}^{v_f(f')} f_Y(y_r) dy_r. \end{aligned} \quad (8.3)$$

The corresponding probability density function could be obtained by the derivative of Eq. (8.3) as

$$f_{F'}(f') = -f_Y(v_f(f')) \cdot v_f'(f'). \quad (8.4)$$

For the special case where the particle is significantly smoother than the surface as that in the following centrifuge experiments, the RMS roughness of particle could be assumed negligible. In this case, $f_{\Sigma_2}(\sigma_2)$ will be a degenerate distribution:

$$f_{\Sigma_2}(\sigma_2) = \begin{cases} 1 & \sigma_2 = 0 \\ 0 & \sigma_2 \neq 0 \end{cases} \quad (8.5)$$

The degenerate distribution of $f_{\Sigma_2}(\sigma_2)$ is not continuous at $\sigma_2 = 0$ and the corresponding distribution of X_2 is

$$f_{X_2}(x_2) = \begin{cases} 1 & x_2 = 0 \\ 0 & x_2 \neq 0 \end{cases}, \quad (8.6)$$

which is also a degenerate distribution. As a result, Eq. (8.2) becomes [256]

$$f_Y(y_r) = f_{X_1}(x_1), \quad (8.7)$$

which means that Y follows the same type of the distribution of X_1 .

The derived mean adhesion force models of van der Waals force (Eq. (7.21) or Eq. (7.22)) and capillary force (Eq. (7.35)) provide the relationship between the force and the sum of the mean square roughnesses, $f' = u_f(y_r)$. Therefore, for every adhesion force, a corresponding y_r could be found and subsequently plugged into Eq. (8.3) to

calculate the cumulative probability of f' . The accumulation of f' and the corresponding cumulative probability will lead to the determination of the adhesion force distribution.

8.2.2 Monte Carlo simulation

Monte Carlo simulation could be employed to model the occurrence of random events. Based on the RMS roughness distribution, Monte Carlo simulation could be used to model the situation that different roughnesses are experienced by the particles when they are deposited onto different sub-areas of a surface, and thus the distribution of adhesion force. The procedure for Monte Carlo simulation-based model is as follows.

(1) During each run of simulation, two random roughnesses, σ_{1ai} and σ_{2ai} ($i=1, 2 \dots N$, is the number of the simulation sequence) are generated from the RMS roughness distributions for the surface and particle, respectively.

(2) Both of these RMS roughnesses are plugged into Eq. (7.1) for the calculation of the effective roughnesses, σ_{1i} and σ_{2i} , which are subsequently substituted into Eq. (7.21) or Eq. (7.22) and Eq. (7.35) for the calculation of van der Waals force and capillary force (if any), respectively. The total adhesion force is calculated as the summation of the van der Waals force and capillary force (Eq. (7.38)).

(3) The above procedure is repeated until all runs of simulation have been finished. The total adhesion force obtained from each simulation run is accumulated to calculate the statistical cumulative probability.

(4) The adhesion force distribution is presented as the relationship between the cumulative probability and the corresponding total adhesion force. The workflow chart of this model is shown by Figure 8.2.

Figure 8.2 The workflow chart of the adhesion force distribution model by the Monte Carlo simulation.

8.3 Validation experiments

8.3.1 RMS roughness measurements

Three types of square-shaped substrate (stainless steel (SS), aluminum (AL) and plastic (PL)) with the size of $3\text{ cm} \times 3\text{ cm}$ were used in the experiments. The relevant mechanical and physical properties for the substrate materials are listed in Table 8.1. For each type of substrate, 4 pieces were prepared and roughed with a file for 1 minute. The roughing of substrates serves to (1) reduce the particle-surface adhesion force to the level which the applicable centrifugal force can afford to overcome, and (2) make the roughness of particles negligible compared to that of substrates. The surface topography of a $15\text{ mm} \times 15\text{ mm}$ area on each piece of substrate which would be deposited with particles in the following centrifuge experiment was scanned by a profilometer (Talyscan 150, Taylor Hobson Ltd.). The surface roughness was obtained by filtering the surface waviness from the scanned topography using the standard cut-off of 0.8 mm. The typical surface roughness characteristic manifested by pseudo-color images for three types of substrate are shown in Figure 8.3. In order to find the RMS roughness distribution for each type of substrate, the RMS roughnesses of 50 randomly located sub-areas ($2\text{ mm} \times 2\text{ mm}$) were read from the scanned area of each substrate. The position coordinates of 50 random points were obtained by using a random number generator. Finally, appropriate probability distributions were fitted to the RMS roughness data of the substrates.

Table 8.1 Mechanical and physical properties of various materials

Materials	Young's modulus (GPa)	Poisson ratio	Surface energy (J/m^2)	Contact angle
PS	4[257]	0.38[257]	0.046[258]	30°[259]
SS	215[260]	0.3[260]	0.007[175]	75°[261, 262]

AL	75.9[263]	0.33[263]	0.25[174]	30°[264, 265]
PL	6[257]	0.35[257]	0.054[176]	10°[266]

Figure 8.3 The surface roughness characteristic for the substrates of (a) stainless steel, (b) aluminum, and (c) plastic, respectively.

The measured cumulative probability data versus the RMS roughness for the substrates of different materials are shown in Figure 8.4. It could be seen that the measured roughness distributions for different substrates of the same material are generally consistent with each other. The plastic substrates are the roughest followed by the aluminum and stainless steel substrates. In order to find out the appropriate statistical distribution for the measured data, 22 non-negative continuous probability distributions were fitted to the data using the software of Easyfit (Mathwave Technologies). The goodness of fit was examined with the test of Kolmogorov-Smirnov, Anderson-Darling and Chi square, respectively. The best fit was the one that had the top average ranking from all three tests and it was found that the gamma distribution provides the best fit towards the measured RMS roughness data. Hence, the gamma distribution is employed for further analysis. The probability density function and cumulative probability function of the gamma distribution are

$$f_{\Sigma_1}(\sigma_1) = \frac{\sigma_1^{\alpha-1} e^{-\frac{\sigma_1}{\beta}}}{\beta^\alpha \Gamma(\alpha)}, \quad (8.8)$$

and

$$F_{\Sigma_1}(\sigma_1) = \frac{\Gamma_{\sigma_1/\beta}(\alpha)}{\Gamma(\alpha)}, \quad (8.9)$$

respectively, where α and β are the shape and scale parameters, respectively. Γ and $\Gamma_{\sigma_1/\beta}$ are the gamma function and incomplete gamma function, respectively. The mean and standard deviation of the gamma distribution are $E(\sigma_1) = \alpha\beta$ and $S(\sigma_1) = \sqrt{\alpha\beta^2}$. Another important statistical parameter is the coefficient of variation (CV) defined as the ratio of the standard deviation to the mean ($S(\sigma_1)/E(\sigma_1)$). CV is a normalized parameter used to measure the dispersion of a probability distribution.

Figure 8.4 The surface RMS roughness data and the corresponding fits of the mean, lower and upper gamma distributions for the substrates of (a) stainless steel, (b) aluminum and (c) plastic, respectively.

For each type of substrate, there are four gamma distributions ($\Gamma(\alpha_i, \beta_i)$, $i = 1, 2, 3, 4$) corresponding to four pieces of substrates. The CV of the fitted roughness distribution ranges from 0.1 to 0.5 for different substrates and a rougher substrate intend to have a larger CV. For each type of substrate, the mean gamma distribution ($\Gamma(\bar{\alpha}, \bar{\beta})$) was obtained by averaging the means and standard deviations of the four individual gamma distributions for the four pieces of substrate. In order to account for the variation of the measured RMS roughness distribution from piece to piece for the same type of substrate, two more gamma distributions are added: one (denoted as the upper gamma distribution: $\Gamma(\bar{\alpha}_+, \bar{\beta}_+)$) is resultant by summing the mean of the mean gamma distribution by two times of its standard deviation; another one (denoted as the lower gamma distribution: $\Gamma(\bar{\alpha}_-, \bar{\beta}_-)$) is resultant by subtracting the mean of the mean gamma distribution by two times of its standard deviation. The shape and scale parameters of the individual gamma distributions ($\Gamma(\alpha_i, \beta_i)$) for each piece of substrate, the mean gamma distribution ($\Gamma(\bar{\alpha}, \bar{\beta})$) and the lower and upper gamma distributions for each type of substrate are listed in Table 8.2. The fitted mean, lower and upper gamma distributions are also shown in Figure 8.4. It could be found that the scope between the lower and upper gamma distributions well covers the measured data.

Table 8.2 Parameters of the gamma distributions.

Material	Substrate No.	Gamma distributions for each substrate		Mean gamma distributions for each material		Upper gamma distributions for each material		Lower gamma distributions for each material	
		α_i	β_i	$\bar{\alpha}$	$\bar{\beta}$	$\bar{\alpha}_+$	$\bar{\beta}_+$	$\bar{\alpha}_-$	$\bar{\beta}_-$
SS	1	10.735	75.426	17.839	48.459	22.895	42.776	13.413	55.885

	2	14.095	60.125						
	3	26.967	35.052						
	4	27.270	31.370						
	1	42.925	28.676						
AL	2	26.489	44.122	23.446	54.611	31.978	46.762	16.236	65.627
	3	9.990	130.430						
	4	37.892	37.449						
	1	21.778	115.650						
PL	2	5.060	441.600	10.356	197.641	20.511	140.437	3.638	333.477
	3	9.989	156.710						
	4	13.127	142.350						

The roughness of the used NIST traceable standards particles (Polysciences, Inc.) is at the order of nanometer [267], which is several orders of magnitude smaller than that of the roughed substrates. Hence, the roughness of particles is assumed negligible. This could also be qualitatively illustrated by the microscopic image of particles on the stainless steel substrate which has the smallest mean RMS roughness (Figure 8.5).

Figure 8.5 The microscopic image of particles on a stainless steel substrate.

8.3.2 Sample preparation

The sample preparation procedure serves to deposit particles onto the substrates to be used for the subsequent centrifuge experiments. All substrates were firstly wiped with tissue paper dipped with ethanol to remove any impurities before being deposited with particles. Since the monodispersed PS particles (size range: $146.1 \pm 1.99 \text{ }\mu\text{m}$) are packaged in a 15mL dropper-tipped bottle with a very high particle concentration, ten drops of suspension from the bottle were mixed with 1 ml de-ionized water for the purpose of dilution. The dilution could moderate the occurrence of aggregation during the following drying process. A pipette (Eppendorf Research plus) was used to dip 40 drops of the diluted liquid onto a designated area ($\sim 1.5 \text{ mm} \times 1.5 \text{ mm}$) of substrate with each drop of $1.5 \text{ }\mu\text{l}$. 40 drops were dipped to allow sufficient particles to be deposited for the statistical accuracy of experiments. Then, the substrates were dried in a forced convection laboratory oven (Esco Isothermo, Model OFA-54-8) at 80°C for 20 hrs [268]. After the drying, the aggregated particles were slowly separated with a needle under the stereomicroscope (Olympus SZX7) and the number (n_0) of particles within the designated area was counted. A total of 2 images were captured side by side to include enough number of particles ($\sim >50$) for accurate statistical analysis, as Ibrahim et al. [260] showed that 30 – 40 particles are needed to produce a statistically accurate result during calculating the fraction of particles resuspended from a surface. The number of particles in each image was counted and summed to give the total number of particles within the designated area.

8.3.3 Centrifuge experiment

8.3.3.1 Centrifuge method

The adhesion force distributions between particles and various types of substrates were measured by the centrifuge method. The centrifuge method adjusts the centrifugal detachment force by changing the rotational speed. This method is a relatively easy way of obtaining the particle-surface adhesion force, especially, the adhesion force distribution, compared to other methods such as atomic force microscopy (AFM) method and electrostatic detachment method [269]. The centrifugal force detaching particles from the surface is given by (Figure 8.6):

$$F_d = m_p \omega_i^2 d \quad (8.10)$$

where $m_p = \frac{4}{3}\pi R_p^3 \rho_p$ is the mass of a single particle of the radius R_p and density ρ_p . $R_p = 73.05 \mu\text{m}$ and $\rho_p = 1050 \text{ kg/m}^3$ for the polystyrene particles used in the experiments. $d = 0.05 \text{ m}$ is the rotational radius. ω_i is the rotational speed which was adjusted in an ascending sequence during the centrifuge experiments. After each rotation (ω_i), the number of particles n_i within the designated area of each substrate was microscopically counted and the fraction of detached particles is calculated by

$$f_r' = 1 - n_i/n_0 \quad (8.11)$$

where n_0 is the initial number of particles within the designated area.

Figure 8.6 A schematic diagram of centrifuge method.

8.3.3.2 Procedure of centrifuge experiment

Four pieces of substrate of the same type from the above sample preparation procedure were vertically secured into the drum rotor (Mikro, Cat. No. 1161) of the centrifuge (Mikro 220R, Cat. No. 2205) by four fabricated adapters (Figure 8.7 (a)). The adapters are made of nylon which allows them to be of great strength and light mass. Each adapter is composed of two separate parts which can be bolted together. The substrate is clamped in-between the two parts. Four adapters were placed into the drum rotor symmetrically as illustrated by Figure 8.7 (b), which helps to maintain the balance of drum rotor. Then, the drum rotor was capped and the centrifuge was switched on to the designated rotational speed for 2 minutes. The duration of 2 minutes is used because the study of Felicetti et al. [67] suggested that a longer duration had no effect on the observed adhesion force from the centrifuge experiments. Since the adhesion force distributions are different for different substrate cases, different arrangements of rotational speed were employed for different substrate cases. For the case of stainless steel substrate, five rotational speeds (3000, 4000, 4500, 5000

and 6000 RPM) were applied. For the case of aluminum substrate, seven rotational speeds (1000, 2000, 3000, 4000, 5000, 6000 and 7000 RPM) were applied. For the case of plastic substrate, seven rotational speeds (1000, 2000, 3000, 4000, 5000, 6000 and 7000 RPM) were applied. The RH and temperature during the experiments were measured to be $85\% \pm 5\%$ and $27 \pm 3\text{ }^{\circ}\text{C}$, respectively, by a RH-temperature sensor (OMEGA, RH-USB).

Figure 8.7 A schematic diagram of (a) an adapter, (b) the centrifuge with four adapters and (c) the centrifuge with the drum rotor capped.

8.3.3.3 Microscopic counting

After each run of centrifuge experiment, the test substrates were microscopically observed to count the number of particles left within the designated area. After finishing the particle counting for each run, the substrates were returned to the centrifuge for the experiment under a closely higher rotational speed followed by another run of particle counting. This procedure was repeated until the particle counting corresponding to the centrifuge experiment of the highest rotational speed has been finished. The fractions of detached particles (Eq. (8.11)) for four pieces of

substrate of the same material were averaged for the model validation. The typical microscopic images after the centrifuge experiments under different speeds are shown by Figure 8.8. It could be seen that the particles are detached by different rotational speeds due to the existence of adhesion force distribution: for the speed of 1000 RPM, only a few particles have been detached, while all particles have been detached for the speed of 7000 RPM.

Figure 8.8 The microscopic image of particles on the plastic substrate after the centrifuge experiments under different rotational speeds: (a) 0 RPM (before the centrifuge experiment); (b) 1000 RPM; (c) 3000 RPM; (d) 5000 RPM; (e) 7000 RPM.

8.4 Results and discussion

8.4.1 Model validation

8.4.1.1 Comparison between model predictions and measurements of this work

Since the predictions from the statistical analysis-based model and the Monte Carlo simulation-based model are similar to each other (See Appendix F), only the predictions from the former are shown during the validation. For each type of substrate, the model predictions are conducted in terms of the mean, lower and upper gamma distributions, respectively. The validation is performed by comparing the

measured adhesion force distributions with the corresponding model predictions as shown in Figure 8.9.

Figure 8.9 The comparison between the measured adhesion force distributions and the modelled ones for particles on the substrates of (a) stainless steel, (b) aluminum and (c) plastic. The error bar indicates one standard deviation. The vertical error bar indicates one standard deviation of measured fraction, while the horizontal error bar indicates the variation of measured adhesion forces caused by the variation of particle size ($146.1 \pm 1.99 \mu\text{m}$), rotational radius ($d \pm 0.01d$) and rotational speed ($\omega_i \pm 0.01\omega_i$).

It is shown in Figure 8.9 that the modeled distributions are generally in good agreement with the experimental ones: both the shape and magnitude of the measured adhesion force distributions are reasonably predicted by the model, validating the proposed adhesion force distribution model. Both the modeling and experimental results show that the median adhesion force is the largest for the stainless steel substrate case followed by the aluminum and plastic substrate cases, respectively. For the dispersion of adhesion force distribution, the case of plastic substrate has the largest one followed by that of aluminum and stainless steel substrates. This should be related to the dispersion of RMS roughness distribution as listed in Table 8.2, where it

has been shown that the plastic substrates have the largest dispersion of RMS roughness distribution followed by the substrates of aluminum and stainless steel, respectively. As an extreme case, it could be expected that there will be no adhesion force distribution for smooth particles contacting with a smooth surface, as there will be no RMS roughness distribution. It should be noted that the variation of the measured fractions indicated by the vertical error bars (Figure 8.9) is generally the smallest for the case of stainless steel substrate among the three cases. This is related to the fact that the roughness variation from piece to piece is the smallest for the case of stainless steel substrate as already shown by Figure 8.4. The horizontal error bars (Figure 8.9) show that there is small measuring error (7%) of the adhesion force due to the variation of particle size, rotational radius and rotational speed.

8.4.1.2 Comparison between model predictions and results of existing study

Further validation is conducted by comparing the model predictions to the experimental data from the study of Prokopovich and Perni [74], where the adhesion force distributions between 60 μm polybutylene terephthalate (PBT) particles and two types of substrates (glass and silicone) were measured. There was no complete RMS roughness distribution data except for the mean RMS roughness. The mean RMS roughnesses for the glass and silicone substrates were 65.78 nm and 43.25 nm, respectively, under the scan size of 4 μm . The standard deviations of the RMS roughness distributions were estimated based on the measurements of this work. As described in Section 8.3.1, the CV of the measured RMS roughness distribution ranges from 0.1 to 0.5 and a rougher substrate intend to have a larger CV. For the model predictions, the CV for the glass and silicone substrates of Prokopovich and

Perni [74] are assigned with 0.2 and 0.1, respectively. The gamma RMS roughness distribution is also employed for the model predictions and the corresponding parameters (α and β) are listed in Table 8.3. Following the original study [74], the roughness of particles is assumed to be negligible compared to that of substrates. The mechanical and physical properties of various materials used for modeling are listed in Table 8.4. The comparison between the model predictions and the experimental data is shown in Figure 8.10.

Table 8.3 Parameters of the gamma roughness distributions for the study of Prokopovich and Perni [74].

Material	α	β
Glass	25.000	2.631
Silicone	69.444	0.610

Table 8.4 Properties of various materials from the study of Prokopovich and Perni [74].

Materials	Young's modulus (GPa)	Poisson ratio	Surface energy (J/m ²)	Contact angle
PBT	0.01	0.4	0.032	93.5°
Glass	50	0.3	0.037	78°
Silicone	7.5×10^{-4}	0.5	0.032	77 °

It can be seen from Figure 8.10 that the measured adhesion force distributions are generally well predicted by the proposed model. For the case of silicone substrate, the model prediction is almost overlapping with the experimental data, suggesting the gamma roughness distribution well describes the actual RMS roughness distribution. For the case of glass substrate, there is slight difference between the measurement and the prediction in the small adhesion force range (2 – 20 nN). Obviously, the measured

adhesion force displays a bimodal distribution as mentioned by the study of Götzinger and Peukert [68] as well. It is speculated that a bimodal roughness distribution may be more appropriate for describing the actual roughness distribution than the employed gamma distribution, meaning that the RMS roughness is not necessarily gamma distributed. However, due to the lacking of relevant information, further analysis in terms of a bimodal roughness distribution is impossible at the moment but left for future study. This finding will not affect the application of the proposed model, because whenever the actual RMS roughness distribution is available, it could be plugged into the model for predicting the adhesion force distribution. It will be important to accumulate the data bank about the RMS roughness distributions for different types of surfaces, which should be a meaningful topic for future study.

Figure 8.10 The comparison of adhesion force distributions between the model predictions and the experimental data of Prokopovich and Perni [74]: (a) glass substrate and (b) silicone substrate.

8.4.2 Effect of RMS roughness distribution on adhesion force distribution

The effect of RMS roughness distribution (the mean and standard deviation of a RMS roughness distribution) on the adhesion force distribution is further explored using the proposed model. This will project useful information for the control of adhesion force relevant processes. The basic case is PS particles on the stainless steel substrates as that in the centrifuge experiments, but the diameter of particle is set to be 150 μm . To study the effect of the mean of RMS roughness distribution, the mean of RMS roughness distribution in the basic case is increased and decreased by 20% and 40%, respectively, while keeping the standard deviation constant. To study the effect of the standard deviation of RMS roughness distribution, the standard deviation of RMS roughness distribution of the basic case is increased and decreased by 20% and 40%, respectively, while keeping the mean constant. All other parameters are the same as those in the basic case (Table 8.1). The adhesion force distributions corresponding to different RMS roughness distributions are shown in Figure 8.11.

Figure 8.11 The variation of adhesion force distributions resultant from the variation of (a) the mean and (b) standard deviation of RMS roughness distribution.

It is shown in Figure 8.11 (a) that the median of adhesion force distribution decreases (or increases) as the increase (or decrease) of the mean RMS roughness. This is consistent with the fact that the adhesion force decreases as the increase of roughness as shown by Eq. (7.21), Eq. (7.22) and Eq. (7.35). The shape of adhesion force distribution scarcely varies as the change of the mean RMS roughness. This suggests that the CV of adhesion force distribution could rarely be affected by the variation of the mean RMS roughness. However, since CV is defined as the ratio of the standard deviation to the mean, the standard deviation of adhesion force distribution decreases as the increase of the mean RMS roughness that leads to the decrease of the mean adhesion force (as indicated by the median). Correspondingly, one extreme case could be expected: the standard deviation of adhesion force distribution will be asymptotic to zero as the surface roughness goes to infinity, leading to zero adhesion force. As a

whole, the mean of RMS roughness distribution could influence both the median and standard deviation of adhesion force distribution.

In Figure 8.11 (b), it is shown that the adhesion force distribution becomes narrower (or wider) as the standard deviation of RMS roughness distribution decreases (or increases). This has also been observed by the previous experimental studies [50, 68, 254]. The significant narrowing (or widening) suggests the decrease (or increase) of the standard deviation of adhesion force distribution. Reasonably, there is the extreme case that the adhesion force distribution has zero standard deviation (i.e., there is only a single value for the adhesion force), when there is no roughness distribution (smooth contact). The median of adhesion force distribution slightly decreases (or increases) as the decreasing (or increasing) standard deviation of RMS roughness distribution. This might be related to the positive skewness of the gamma roughness distribution which increases when the standard deviation increases and the mean keeps constant. The increase of skewness means that the probability for the occurrence of small roughness would be higher, which increases the occurrence probability of large adhesion forces and thus the median adhesion force. Hence, the median adhesion force will increase as the increase of the standard deviation of RMS roughness distribution. In conclusion, both the median and standard deviation of adhesion force distribution could be affected by the RMS roughness distribution (the mean and standard deviation).

8.5 Conclusions

In this chapter, a model for the adhesion force distribution between particles and the surface has been proposed by integrating the RMS roughness distribution into the

mean adhesion force models of Chapter 7. The integration was performed by the statistical analysis and Monte Carlo simulation, respectively. The validation of the proposed model was accomplished by comparing the measured adhesion force distributions from a series of centrifuge experiments and the existing study to the model predictions and a good agreement has been found. The influence of the RMS roughness distribution towards the adhesion force distribution was analyzed based on the proposed model. It was found that both the median and standard deviation of adhesion force distribution could be affected by the mean and standard deviation of RMS roughness distribution, respectively, meaning that controlling adhesion force distribution could be practically achieved by adjusting the mean or standard deviation of RMS roughness distribution. Unlike the existing models, this model could predict both van der Waals force and capillary force distributions, greatly extending the current capability of adhesion force distribution prediction.

Chapter 9 A New Theoretical Model for AIPR

9.1 Introduction

It could be identified that the process of AIPR actually bears some fundamental characteristics by examining the hydrodynamic detachment forces, adhesion force and physical phenomena of the process. These fundamental characteristics should be considered for the development of a physically reasonable AIPR model.

Turbulent flow always exists in indoor environments and ventilation ducts [30, 31]. As reviewed in Chapter 2, existing studies (e.g., [81, 83]) have shown that turbulent flow is continually erupting with turbulent bursts leading to an unsteady boundary layer inside. The occurrence of turbulent bursts intends to modify the hydrodynamic detachment forces experienced by particles and thus influence the particle resuspension process. Consequently, turbulent bursts should be taken into consideration by the resuspension model to reflect the underlying fluid mechanics of the process. Meanwhile, the occurrence of turbulent bursts generally follows a certain spatial and temporal intervals, which allows for the mathematical consideration of turbulent bursts.

Both particles and surfaces are rough in real scenarios of indoor environment and ventilation duct. In this case, the adhesion force between particles and a surface will follow a distribution rather than be a single value [50, 67-76] as described in Chapter 8. The existence of adhesion force distribution means that some particles tightly adhered to the surface are more difficult to be resuspended, while some other particles

lightly adhered to the surface are easier to be resuspended. This partly contributes to the phenomenon that some particles are resuspended leaving others to remain on the surface during the process. Furthermore, as particle resuspension proceeds, more and more particles are detached from the surface, leaving the ones that are more and more difficult to be resuspended, that is, the amount of resuspendable particles on the surface is gradually depleted. This matter of fact has been referred as the “harvesting effect” by [119] and is phenomenally reflected by the decay of resuspension rate with respect to time during the process [109, 270, 271]. Therefore, the physical phenomenon behind AIPR cannot be appropriately captured without taking the adhesion force distribution and the depletion of resuspendable particles into consideration.

In indoor environments and ventilation ducts, water vapour could condense at the interface between particles and a surface and form menisci, when the environmental RH is high enough (higher than the critical RH) [30, 63, 272] as shown in Chapter 7. The capillary forces will be induced due to the formation of menisci, which will affect the total adhesion forces between the particles and surface and thus the particle resuspension process. Generally, the capillary force between a particle and surface varies as RH, when the environmental RH is larger than the critical one. This means that the influence of the induced capillary force towards AIPR depends on the RH level. Considering the variability of RH in real environments, the capability of predicting the effect of RH (capillary force) will be crucial for the practical application of an AIPR model.

On the whole, the essential characteristics underlying AIPR could be summarized as: (1) turbulent bursts play an important role for particle resuspension; (2) the adhesion force between particles and a surface follows a distribution and the amount of resuspendable particles will be depleted as resuspension progresses; (3) environmental RH is closely related to the capillary force and thus the particle resuspension process. Despite the characteristics underlying the process, the existing models fail to take one or several of them into consideration as reviewed in Chapter 2. In this chapter, a turbulent burst-based model was proposed with the consideration of the depletion of resuspendable particles on the surface, the adhesion force distribution and the effect of RH. The model would significantly extend the current capability of modelling AIPR theoretically. The validation of the proposed model was accomplished by comparing existing experimental data to model predictions.

9.2 Model development

9.2.1 Detachment mode of resuspension

Generally, it was regarded that there were three detachment modes for AIPR: lift-off, sliding and rolling. The study of Wang [273] suggested that particles could be most easily detached by the mode of rolling for resuspension. Several other studies [274, 275] further validated that the mode of detachment is rolling rather than sliding and lift-off. Hence, rolling is adopted as the detachment mode in this work. According to the moment balance, as shown in Figure 9.1, the detachment criterion for the rolling mode is

$$1.4R_p F_D + aF_L \geq a(F_A + F_G), \quad (9.1)$$

where F_D , F_L , F_A and F_G are the hydrodynamic drag, hydrodynamic lift, adhesion force and gravitational force, respectively. R_p is the particle radius. a is the contact radius. The drag force acts at $y = 1.4R_p$ considering the non-uniformity of the flow field [97]. Based on Eq. (9.1), the critical detachment force is defined as

$$F_{cA} = \frac{1.4R_p F_D}{a} + F_L - F_G. \quad (9.2)$$

When the adhesion force between the particle and surface is smaller than the critical detachment force, the particle will be detached.

Figure 9.1 A schematic diagram of the rolling detachment mode.

9.2.2 Hydrodynamic and adhesion forces

9.2.2.1 Hydrodynamic forces

According to the wall law of turbulent boundary layer, the relationship between the mean non-dimensional velocity u^+ and the non-dimensional height y_h^+ in the viscous sublayer is given by Eq. (2.4) in Chapter 2. The mean non-dimensional velocity is substituted into the lift and drag force models to calculate the mean hydrodynamic forces.

Turbulent bursts lead to the formation of streaks in the viscous sublayer and make the viscous sublayer unsteady [83]. The airflow velocity will be modified in the case of turbulent bursts, which results in the fluctuation of the hydrodynamic forces experienced by particles. The relationship between the non-dimensional instantaneous velocity u_t^+ and non-dimensional height y_h^+ during a turbulent burst-sweep event is given by Eq. (2.8) in Chapter 2. The instantaneous velocity is used in the lift and drag force models to calculate the instantaneous hydrodynamic forces.

The lift force is calculated using the model from [95] or [96] as shown by Eq. (2.9) in Chapter 2. The drag force model has been derived by O'Neill (1968) as shown by Eq. (2.10) in Chapter 2.

9.2.2.2 Adhesion force distribution

As reviewed in Chapter 2, the van der Waals force and capillary force serve as the major interaction forces for submicron-sized or micron-sized particles as considered in indoor particle exposure analysis. Due to the existence of roughness distribution, there is an adhesion force distribution between particles and a surface, which will affect the particle resuspension process. The adhesion force distribution model has been developed in Chapter 8 by integrating the RMS roughness distribution into the mean adhesion force models of Chapter 7. This model is capable of predicting both van der Waals force and capillary force distributions. Applying this model for AIPR modelling allows the effect of RH to be considered. Considering that the predictions from the statistical analysis-based model and the Monte Carlo simulation-based model

are similar to each other, only the Monte Carlo simulation-based model is applied here. The predicted adhesion force distribution is presented as the relationship between the cumulative probability and the corresponding total adhesion force. A typical cumulative probability distribution of adhesion force is shown by Figure 9.2. More details about the adhesion force distribution model are shown in Chapter 7 and Chapter 8 and are not repeated here.

Figure 9.2 The cumulative distribution of adhesion force between particles and a surface.

9.2.2.3 Gravitational force

The gravitational force for a particle is given by

$$F_G = m_p g, \quad (9.3)$$

where m_p is the mass of a particle. $g = 9.81 \text{ m/s}^2$ is the gravitational acceleration.

For submicron-sized and micron-sized particles, the gravitational force is actually

negligible in Eq. (9.1), since it is generally two to three orders of magnitude smaller than the adhesion force. But it is still considered here for the purpose of completeness.

9.2.3 Principle of resuspension model

In turbulent flow, turbulent bursts are distributed fairly uniformly with a certain non-dimensional spanwise and longitudinal spacings λ_s^+ and λ_l^+ , and occurred with a certain non-dimensional period T^+ . According to Table 2.1, the non-dimensional spanwise spacing, longitudinal spacing and period between bursts are:

$$\begin{aligned}\lambda_s^+ &= \frac{\lambda_s u^*}{\eta} = 100, \\ \lambda_l^+ &= \frac{\lambda_l u^*}{\eta} = 630 \quad \text{and} \\ T^+ &= \frac{T u^{*2}}{\eta} = 80.\end{aligned}\tag{9.4}$$

Similar to the study of Cleaver and Yates [99], a circular area of the radius, $r' = \frac{10\eta}{u^*}$, is used to denote the scope that one burst can affect and a rectangular area of the dimensions $\lambda_s \times \lambda_l$ is used as the control area where bursts occur randomly in space and periodically per T^+ (Figure 9.3). In order to model the occurrence of turbulent bursts in the control area, Monte Carlo simulation is carried out. The spanwise and longitudinal positions of new bursts are determined by a random number generator: a random number between 0 and 1 was firstly generated and then multiplied by the spanwise and longitudinal spacing to calculate the position coordinates.

Figure 9.3 A schematic diagram of turbulent bursts in the model.

Without the occurrence of turbulent burst, particles will experience the mean hydrodynamic forces that lead to the critical detachment force F_{CA1} (Eq. (9.2)) corresponding to the cumulative probability, P_1 , in the adhesion force distribution as illustrated in Figure 9.2. This means that the fraction, P_1 , of particles have the adhesion forces smaller than the critical detachment force, F_{CA1} , and thus will be resuspended. Once these particles are resuspended from the surface, they are depleted and no longer available for further resuspension. When a turbulent burst occurs, particles will experience the instantaneous hydrodynamic forces that lead to the critical detachment force F_{CA2} ($F_{CA2} > F_{CA1}$) (Eq. (9.2)) corresponding to the cumulative probability, P_2 , in the adhesion force distribution (Figure 9.2). In this case, the fraction, $(P_2 - P_1)$, of particles in the circular area of $\frac{\pi}{4} \left(\frac{20\eta}{u^*} \right)^2$ will be resuspended. However, when the new burst overlaps with the previous bursts, there will be no particle resuspension within the overlapping area where the particles have been depleted; that is, there is only particle resuspension within the newly occupied area by the new burst. Hence, the newly occupied area needs to be modeled.

When the new burst overlaps with only one previous burst, the newly occupied area can be calculated as (Figure 9.4 (a))

$$S_n = \pi r'^2 - S_o = \pi r'^2 - (2r'^2 \cos^{-1} \frac{L}{2r'^2} - L\sqrt{r'^2 - \frac{L^2}{4}}), \quad (9.5)$$

where S_o is the overlapping area and L is the distance between the centers of two bursts. However, when the new burst overlaps with 2 or more than 2 previous bursts (Figure 9.4 (b)), some of which might also overlap with each others, the calculation of the newly occupied area is a prohibitive traversal problem. In this instance, a simplified calculation is conducted as

$$S_n = \pi r'^2 - S'_o = \begin{cases} \pi r'^2 - S'_o & (\pi r'^2 - S'_o) \geq 0 \\ 0 & (\pi r'^2 - S'_o) < 0 \end{cases}, \quad (9.6)$$

where S'_o is the sum of individual area that the new burst overlaps with each previous burst calculated based on S_o in Eq. (9.5). Considering that a large number of bursts occur during the resuspension process, the adverse effect from this simplification is believed to be averaged and small.

Figure 9.4 A schematic diagram of overlapping bursts. (a) The new turbulent burst overlaps with only one previous burst. (b) The new turbulent burst overlaps with 2 or more than 2 previous bursts. Circles 1 and 1' indicate the areas occupied by the previous bursts. Circles 2 indicate the areas occupied by the new burst. Newly occupied area is highlighted by the red shadow lines.

The procedure of the resuspension model is summarized as follows.

- (1) When the airflow is initiated, the fraction, P_1 , of particles which have the adhesion forces smaller than F_{cA1} corresponding to the mean airflow velocity, Eq. (2.4), will be resuspended. These particles are depleted from the surface and are no longer available for further resuspension.
- (2) A turbulent burst randomly occurs in the control area. It resuspends the fraction, $(P_2 - P_1)$, of particles in the circular area of $\frac{\pi}{4}(\frac{20\eta}{u^*})^2$. The resuspended particles have the adhesion forces larger than F_{cA1} but smaller than F_{cA2} corresponding to the instantaneous flow velocity, Eq. (2.8). Once resuspended, they are no longer available for further resuspension as well.
- (3) After a period of T , a new burst randomly occurs again in the control area. If this burst occupies some new area, that is, there are some areas that the new burst does not overlaps with the previous bursts, the fraction, $(P_2 - P_1)$, of particles within this new area will be resuspended. These particles also have the adhesion forces larger than F_{cA1} but smaller than F_{cA2} . This process will be repeated per period of T until the time of simulation is up.

9.3 Results

9.3.1 Model validation

The experimental data from existing studies [212, 260, 274] are adopted for the model validation. In the studies of Ibrahim et al. [260, 274], the experimental data were presented as the detachment fraction (fraction of particles resuspended) with respect

to the free stream velocity, while the experimental data were presented as the threshold velocity with respect to the particle diameter in the study of Ibrahim et al. [212]. Hence, the model validation is performed in terms of these two types of experimental results, respectively.

9.3.1.1 Detachment fraction versus free stream velocity

In the study of Ibrahim et al. [274], 70 μm stainless steel particles (SS70), 32 μm and 72 μm glass particles (GL32 and GL72) were resuspended from the glass substrate (GL) under the RH of 25%. Whereas, in the study of Ibrahim et al. [260], 70 μm stainless steel (SS70) particles were resuspended from the glass substrate under the different RHs (36%, 61% and 67%). The mechanical and physical properties for the materials of the particles and substrate are listed in Table 9.1. The RMS roughness of glass substrate has been measured using an atomic force microscope (AFM) under the scan length of 20 μm . The measured RMS roughness of glass substrate ranged from 1.08 to 13.7 nm and could be fitted by the gamma distribution with the shape parameter $\alpha = 1.954$ and the scale parameter $\beta = 0.869$. The measured roughness data and the corresponding gamma distribution are shown by Figure 9.5. The roughness information of particles were not given in the original studies [260, 274]. The RMS roughness of particles is assumed to be gamma distributed as well for the modelling. The estimation of the mean RMS roughness (μ_r) for different particles is based on other existing studies [276, 277] which measured the roughness of micron-sized particles. The estimation of the standard deviation of RMS roughness distribution (σ_r) for different particles is based on the standard deviation of the RMS roughness distribution for the glass substrate. The shape and scale parameters (α and

β), the mean (μ_r) and standard deviation (σ_r) for the gamma roughness distributions of different particles are listed in Table 9.2.

Figure 9.5 The measured RMS roughness data and the corresponding fit of the gamma distribution.

Table 9.1 Mechanical and physical properties of the materials of particle and substrate in the studies of [212, 260, 274].

Material	Density (kg/m ³)	Poisson ratio	Young's modulus (GN/m ²)	Surface energy (J/m ²)	Contact angle (°)
GL	2420	0.22	69	0.2	60
SS	8000	0.3	215	0.3	80

Table 9.2 Parameters of the gamma distributions for various particles in the studies of [212, 260, 274]

Particle	α	β	μ_r (nm)	σ_r (nm)
SS70	1.978	2.276	4.5	3.2
GL32/30.1	26.694	0.116	3.1	0.6

GL52.6	2.403	1.290	3.1	2
GL72/72.6	2.531	1.383	3.5	2.2
GL90.3	4	1.2	4.8	2.4
GL111	4	1.3	5.2	2.6

The predicted adhesion force distributions from the Monte Carlo simulation-based model (Chapter 8) for various cases could be fitted by the lognormal distributions whose parameters are listed in Table 9.3. The lognormal adhesion force distribution between particles and a surface has also been found in the previous experimental studies [67-70, 72]. The adhesion force distributions for various cases are shown in Figure 9.6. It is seen from Table 9.3 and Figure 9.6 that the mean adhesion force of GL72/GL is larger than that of SS70/GL. Despite the significantly smaller particle size, the mean adhesion force of GL32/GL is similar to that of GL72/GL, which is due to that the roughness for GL32 is smaller than that of GL72 as shown by Table 9.2. The smaller dispersion of the adhesion force distribution for GL32/GL than GL72/GL corresponds to the smaller standard deviation of the RMS roughness distribution for 32 μm particles (Table 9.2). The mean adhesion force of SS70/GL increases significantly as the RH due to the increase of capillary force.

Table 9.3 The parameters of adhesion force distributions for various cases in [212, 260, 274].

Particle/Substrate	RH	μ_{adh}	σ_{adh}
SS70/GL	25%	5.3117	0.90954
GL32/GL	25%	5.7332	0.43979
GL72/GL	25%	5.7239	0.91914
SS70/GL	36%	5.4324	0.94766
SS70/GL	61%	6.8934	1.108
SS70/GL	67%	7.5398	0.9882

GL30.1/GL	29%	5.9349	0.50109
GL52.6/GL	29%	6.0334	1.0089
GL72.6/GL	29%	5.8317	0.86645
GL90.3/GL	29%	5.4307	0.61675
GL111/GL	29%	5.4829	0.59231

Figure 9.6 The lognormal adhesion force distributions for (a) 70 μm stainless steel particles, 32 μm and 72 μm glass particles on the glass substrate under the RH of 25% [274]; (b) 70 μm stainless steel particles on the glass substrate under the RH of 36%, 61% and 67%, respectively [260].

During the resuspension modelling, the relationship between the free stream velocity and friction velocity was $u^* = 0.0375U_\infty + 0.0387$ and the particle surface concentration was $5 \times 10^6 \text{ \#}/\text{m}^2$ according to the original studies [260, 274]. The comparison of the detachment fraction versus the free stream velocity between the experimental data and the model predictions is shown by Figure 9.7.

Figure 9.7 The comparison between the experimental data and the model predictions for (a) 70 μm stainless steel particles, 32 and 72 μm glass particles on the glass substrate under the RH of 25% [274]; (b) 70 μm stainless steel particles on the glass substrate under the RH of 36%, 61% and 67%, respectively [260].

It is shown by Figure 9.7 that the model predictions are in good agreement with the experimental data. The sigmoid-shaped relationship between the detachment fraction and the free stream velocity has been well captured by the model. In Figure 9.7 (a), the resuspension of GL72/GL is generally more difficult than that of SS70/GL, which is consistent with the fact that the overall adhesion force for the case of GL72/GL is larger than that for the case of SS70/GL as shown in Figure 9.6. Figure 9.7 (a) also shows that the resuspension is significantly more difficult for the case of GL32/GL than GL72/GL. On the basis of the proposed model, the significantly smaller diameter of GL32 than GL72 leads to both the smaller detachment force and lever arm, which results in the even smaller detachment moment (Eq. (9.1)). As a result, the detachment fraction will be much smaller for the case of GL32/GL than that for the case of GL72/GL at the same free stream velocity. In Figure 9.7 (b), the particle resuspension becomes more and more difficult as the RH increases. This corresponds to the increase of total adhesion force (Figure 9.6 (b)) due to the increase of capillary force when the RH increases. Hence, the influence of RH towards AIPR has been reasonably predicted by the model, which has rarely been achieved by the existing AIPR models.

9.3.1.2 Threshold friction velocity versus particle size

The threshold friction velocity is defined as the friction velocity necessary to detach 50% of particles on the surface in [212] which measured the threshold velocities for the glass particles of diameter 30.1 (GL30.1), 52.6 (GL52.6), 72.6 (GL72.6), 90.3 (GL90.3) and 111 (GL111) μm on the glass substrate. The RMS roughness distribution of the glass substrate is the same as that shown in Figure 9.5. The RMS

roughness distributions for various glass particles were not given and are assumed to be gamma ones as well whose parameters are listed in Table 9.2. The RMS roughness distributions for GL30.1 and GL72.6 are set to be the same as that for the above GL32 and GL72, considering their similar diameters, respectively. The predicted adhesion force distributions for different particles could also be fitted by the lognormal distributions (Figure 9.8) whose parameters are listed in Table 9.3. The particle surface concentration in the experiments was $5 \times 10^5 \text{ \#/m}^2$ and the RH was 29% according to the original study [212]. Other relevant parameters are listed in Table 9.1. The comparison between the model predictions and experimental data is shown in Figure 9.9. For better comparison, a power law trend-line is fitted to the model predictions.

Figure 9.8 The lognormal adhesion force distributions for various cases in the study of [212].

It is shown in Figure 9.9 that the model predictions are consistent with the experimental data. The decreasing trend of threshold friction velocity with respect to the particle diameter is successfully captured by the model, which further validates the proposed model. The declination of threshold velocity versus the particle diameter is mainly due to the fact that the hydrodynamic forces (Eq. (2.9) and Eq. (2.10)) are at least second order proportional to the particle size, while the adhesion forces (Eq. (7.21), Eq. (7.22) and Eq. (7.35)) are only first order proportional to the particle size. This means that the ratio between the detachment forces and adhesion forces is higher for larger particles. As a result, the larger particles would be more easily detached than the smaller ones; that is, larger particles correspond to smaller threshold friction velocities.

Figure 9.9 The comparison between the experimental data of [212] and the model predictions.

9.4 Conclusions

A new theoretical AIPR model has been developed with the following considerations: (1) turbulent bursts play an important role for particle resuspension; (2) the adhesion force between particles and a surface follows a distribution due to the existence of surface roughness and the resuspendable particles will be depleted as resuspension progresses; (3) environmental RH could affect AIPR via the induced capillary force. The Monte Carlo simulation was performed to model the occurrence of turbulent bursts and the depletion of resuspendable particles. The employment of the adhesion force distribution model developed in Chapter 8 allows the adhesion force distribution and RH effect to be considered. The model validation was accomplished by comparing the model predictions with the existing experiment data (detachment fraction vs. free stream velocity and threshold friction velocity vs. particle diameter) and a good agreement was found. The proposed model provides a physically reasonable framework for describing AIPR. Especially, the ability of predicting the RH effect greatly enhances the current capability of modelling AIPR practically.

Chapter 10 Conclusions and Suggestions for Future Work

10.1 Conclusions

Deposited pathogens could be resuspended by airflow or mechanical disturbances and become airborne again, leading to the prolonged inhalational exposure risk. Hence, pathogen resuspension can serve as a possible route for infection transmission. Understanding the impact of resuspension on infection transmission is crucial for developing a complete risk assessment scheme. This work serves to improve the current capability of modelling resuspension processes and explore the impact of the resuspension processes on infection transmission.

Particle resuspension is governed by the interaction between particle-surface adhesion forces and detachment forces. Depending on the detachment forces, there are two common types of particle resuspension process related to indoor environments: airflow-induced particle resuspension (AIPR) and walking-induced particle resuspension (WIPR), both of which were investigated in this work.

The particle resuspension in the ventilation duct in the case of a bioterrorist attack was explored as a major AIPR case relevant to infection transmission. The corresponding particle concentration dynamics model was developed based on the existing empirical AIPR models and validated by the experimental data from wind tunnel experiments. It was found that the particle concentration increased immediately after the initiation of airflow in the duct and gradually decreased as the time went on. The spatial particle concentration variation along the duct after resuspension was also explored based on

the proposed model. The concentration increased downstream until reaching a critical point after which the concentration dropped sharply to the background level. The proposed model serves as the foundation for predicting the pathogen concentration in the ventilation duct with AIPR and in the occupied space.

In the case of WIPR, a scaled resuspension chamber into which a pair of model feet was installed was fabricated. The resuspension rate during the simulated walking activities was calculated based on the mass balance model and the power law was applied to fit the resuspension rate data. The resuspension rate was further normalized for investigating the effects of various factors (e.g., flooring material, particle size, walking rate, RH and mechanism) on WIPR. It was found that the normalized resuspension rate of PM_{10} was about 2.5 times that of $PM_{2.5}$ for both carpet and wood PVC. Carpet had the highest resuspension rate, followed by wood PVC and vinyl. The reduction of normalized resuspension rate due to the lower walking rates was less significant for carpet than for vinyl. The normalized resuspension rate under the low RH (42%) was significantly higher than the rates under the higher RH (63% and 82%). The normalized resuspension rate is much smaller in the aerodynamic case than in the contact case, indicating that the addition of mechanical mechanism is critical for WIPR. The time-dependence of the resuspension rate of WIPR roughly follows the power law. The power exponent b_r ranged from 0.42 to 0.79 with the mean and standard deviation of 0.62 and 0.11, respectively, for WIPR. Based on the power law relationship, an airborne particle concentration model has been developed. The developed model could predict the overall variation of airborne particle concentration involved with human walking. The method adopted for deriving the model provides a

hint for developing the more integrative indoor airborne and surface particle concentration models.

The model of particle concentration dynamics in the ventilation duct with AIPR and the power law resuspension rate for WIPR were then substituted into the mass balance models of indoor particle dynamics to develop a set of airborne and surface particle concentration models. The contributions of AIPR and WIPR towards indoor particle dynamics could be clearly identified based on the developed models. The developed models serve as the basis for the pathogen exposure analysis and thus risk assessment.

A set of inhalational exposure analysis models was developed based on the proposed indoor particle concentration models. A risk assessment scheme of infection transmission was proposed by integrating the exposure analysis into the dose response model. This scheme is capable of quantifying the effect of pathogen resuspension on infection transmission. The impact of resuspension on infection transmission was examined by studying two hypothetical cases on bioterrorist attack. In the case about ventilation systems-based attack, the AIPR served to prolong occupants' exposure to BW pathogen. In this case, the WIPR could significantly affect the infection probability only if a large amount of pathogens were dosed and the walking started long time after the resuspended pathogens enter indoors so that there were enough pathogens on the floor for the WIPR. In the case that pathogens were placed on the indoor floor by the attack, the WIPR could lead to both prolonged exposure and high infection probability. Early identification of the bioterrorist attack and evacuation of occupants were found to be critical for effectively mitigating the attack in this case.

Further effort was put to develop an improved theoretical AIPR model which has the potential to be used in exposure modelling in the future. The mean adhesion force models were firstly developed by considering the characteristic of multiple roughness scales with the fractal theory and the Gaussian roughness distribution. The new models were validated against the existing experimental data, showing good agreement. The new models converge to the classical solutions for the contact between a smooth spherical particle and a surface. On the basis of the new models, the influences of roughness, RH, contact angle and Hurst exponent towards mean adhesion forces were investigated. The decline mode of adhesion force with surface roughness and contact angle as well as the increase mode with RH and Hurst exponent observed previously can now be reasonably explained by the new models. The comparison between the models of this work and the existing studies was performed during the parameter investigations in terms of roughness, RH and contact angle, respectively. The models of this work identify the fact that the RMS roughness is scan length dependent and consider the effect of roughness together with the corresponding scan length based on the fractal theory, which has been rarely achieved by the existing models.

The model of adhesion force distribution between particles and a surface was then proposed by integrating the RMS roughness distribution into the developed mean adhesion force models. The integration was performed by the statistical analysis and Monte Carlo simulation, respectively. The validation of the proposed model was accomplished by comparing the model predictions with the measured adhesion force distributions from a series of centrifuge experiments and the existing study. The influence of RMS roughness distribution towards the adhesion force distribution was

analyzed based on the proposed model. It was found that both the median and standard deviation of adhesion force distribution could be affected by the mean and standard deviation of RMS roughness distribution, respectively. This means that controlling adhesion force distribution could be practically achieved by adjusting the RMS roughness distribution. Unlike the existing models, this model is able to predict both van der Waals force and capillary force distributions, greatly extending the current capability of modeling adhesion force distribution.

The adhesion force distribution model was then applied during the development of the new theoretical AIPR model which considers some essential characteristics underlying AIPR (i.e., turbulent burst, adhesion force distribution, depletion of resuspendable particles and RH). The Monte Carlo simulation was performed to model the occurrence of turbulent bursts and the depletion of resuspendable particles. The model validation was accomplished by comparing the model predictions to the existing experiment data (detachment fraction vs. free stream velocity and threshold friction velocity vs. particle diameter). The proposed model provides a physically reasonable framework for describing AIPR. The ability of predicting the RH effect on AIPR greatly enhances the current capability of modelling AIPR practically.

10.2 Suggestions for future study

Despite the above work accomplished, some more studies are still needed to complete the understanding about resuspension and its impact on infection transmission.

(1) The deposited particles as considered in Case 2 (section 6.4.2) may interact with the existing particles on the floor, which may affect the actual resuspension rate for the introduced particles. Future study is suggested to explore the potential effect of existing particles on the resuspension of newly introduced particles.

(2) The developed adhesion force (distribution) models are applicable for the contact between rough spherical particles and a surface. Considering that the shape of pathogens is not limited to sphere, future study is suggested to combine the shape effect into the developed models of this work. This may be achieved by comparing the experimentally determined adhesion forces between non-spherical particles and a surface with the model predictions of this work and introducing a shape factor for correction.

(3) The existing models of hydrodynamic forces are applicable for spherical particles. It will be desirable to develop the hydrodynamic force models for non-spherical particles, which can also be done by introducing a shape correction factor into the existing models according to experimental or numerical analysis.

(4) Considering the possible effect of plastic deformation on the adhesion force between particles and a surface, it will be desirable to model this effect on adhesion forces in the future. This will definitely contribute to complete our understanding about the adhesion phenomena between particles and a surface.

(5) The adhesion force distribution model is based on the concept of RMS roughness distributions of particles and surfaces. Different types of surfaces (particles) may have

different types of RMS roughness distribution. Hence, further exploration about the relationship between the type of surface and the type of RMS roughness distribution will be beneficial for the model application in the future.

(6) The developed AIPR model has the potential to be used in exposure modeling. This can be achieved by combining the developed AIPR model with the CFD simulation of airflow field.

(7) The developed airborne concentration models are based on the well mixed assumption. Two methods are suggested in the future to handle the case where the well mixed assumption does not hold. The first method is to divide indoor space into smaller zones which the well-mixed assumption and thus the developed models are applicable for. Then, these different zones are related to each other by Markov chain model [200]. The second method is to integrate the AIPR model and the resuspension rate of WIPR into the CFD simulation of indoor particle dynamics.

Appendix A. Derivation of Eq. (3.4)

The governing equation is

$$A_v \frac{\partial C_{ov}(x,t)}{\partial t} + Q_s \frac{\partial C_{ov}(x,t)}{\partial x} = -V_d C_{ov}(x,t) P_v \quad (A.1)$$

under the boundary condition of

$$C_{ov}(x,t)|_{x=0} = C_0 + \frac{N_0 S_v r_{n1} t^{-r_{n2}}}{Q_s} \quad (A.2)$$

and the initial condition of

$$C_{ov}(x,t)|_{t=0} = C_{t0}. \quad (A.3)$$

Making a coordination transformation to t and x with $\xi = t$ and $\eta = Q_s t - A_v x$, and

having $\omega(\xi, \eta) = C_{ov}(x(\xi, \eta), t(\xi, \eta))$ yield

$$\frac{\partial C_{ov}}{\partial t} = \frac{\partial \omega}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial \omega}{\partial \eta} \frac{\partial \eta}{\partial t} = \frac{\partial \omega}{\partial \xi} + Q_s \frac{\partial \omega}{\partial \eta} \quad \text{and} \quad (A.4)$$

$$\frac{\partial C_{ov}}{\partial x} = \frac{\partial \omega}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial \omega}{\partial \eta} \frac{\partial \eta}{\partial x} = -A_v \frac{\partial \omega}{\partial \eta}. \quad (A.5)$$

Based on Eq. (A.4) and Eq. (A.5), Eq. (A.1) will become

$$\frac{\partial \omega}{\partial \xi} + \frac{V_d P_v}{A_v} \omega = 0, \quad (A.6)$$

which can be further changed to

$$\frac{\partial}{\partial \xi} \left(e^{\frac{V_d P_v}{A_v} \xi} \omega \right) = 0. \quad (A.7)$$

Integrating Eq. (A.7) with respect to ξ results in

$$e^{\frac{V_d P_v}{A_v} \xi} \omega = f(\eta) \quad (A.8)$$

which gives

$$\omega = f(\eta) e^{-\frac{V_d P_v}{A_v} \xi}. \quad (A.9)$$

Substituting $\xi(x, t)$ and $\eta(x, t)$ back into Eq. (A.9) leads to

$$C_{ov}(x, t) = f(Q_s t - A_v x) e^{-\frac{V_d P_v}{A_v} x}. \quad (A.10)$$

Based on the boundary condition, Eq. (A.2), the differentiable function $f(Q_s t - A_v x)$ in Eq. (A.10) can be defined and Eq. (A.10) becomes

$$C_{ov}(x, t) = \frac{N_0 S_v r_{n1}}{Q_s(t - \frac{A_v x}{Q_s}) r_{n2}} e^{-\frac{V_d P_v x}{Q_s}} + C_0 e^{-\frac{V_d P_v x}{Q_s}}. \quad (A.11)$$

Obviously, if $t \leq \frac{A_v x}{Q_s}$, Eq. (A.11) will become unreasonable. Actually, when $t \leq \frac{A_v x}{Q_s}$, the location x will not be affected by the particle resuspension and upstream concentration C_0 . Considering the initial condition, Eq. (A.3), the solution of Eq. (A.1) should be finalized as

$$C_{ov}(x, t) = \begin{cases} C_{t0} & (0 < t \leq \frac{A_v x}{Q_s}) \\ \frac{N_0 S_v r_{n1}}{Q_s(t - \frac{A_v x}{Q_s}) r_{n2}} e^{-\frac{V_d P_v x}{Q_s}} + C_0 e^{-\frac{V_d P_v x}{Q_s}} & (\frac{A_v x}{Q_s} < t) \end{cases}. \quad (A.12)$$

Appendix B. Derivation of Eq. (7.13)

The Gaussian distribution is

$$p_h = \frac{1}{(2\pi)^{1/2}\sigma} e^{-h^2/(2\sigma^2)} . \quad (\text{B.1})$$

The combined roughness distribution is obtained by the convolution of p_{h1} and p_{h2} as:

$$P_h(h) = \int_{-h_{\min 1}}^{h_{\max 1}} p_{h1}(h_1) p_{h2}(h - h_1) dh_1 = \int_{-h_{\min 2}}^{h_{\max 2}} p_{h1}(h_2) p_{h2}(h - h_2) dh_2 , \quad (\text{B.2})$$

where p_{h1} and p_{h2} are the Gaussian roughness distributions of the two contacting surfaces. $h_{\min 1}$, $h_{\max 1}$, $h_{\min 2}$ and $h_{\max 2}$ are the maximum height of peak and maximum height of valley for the two contacting surfaces. Substituting the Gaussian distribution into Eq. (B.2) yields

$$P_h(h) = \int_{-h_{\min 1}}^{h_{\max 1}} \frac{1}{(2\pi)^{1/2}\sigma_1} e^{-h_1^2/(2\sigma_1^2)} \cdot \frac{1}{(2\pi)^{1/2}\sigma_2} e^{-(h-h_1)^2/(2\sigma_2^2)} dh_1 = \frac{1}{2\pi\sigma_1\sigma_2} \int_{-h_{\min 1}}^{h_{\max 1}} e^{-(\sigma_2^2 h_1^2 + \sigma_1^2 h^2 - 2\sigma_1^2 h h_1 + \sigma_1^2 h_1^2)/(2\sigma_1^2 \sigma_2^2)} dh_1 = \frac{1}{2\pi\sigma_1\sigma_2} e^{-h^2/(2\sigma_2^2)} \int_{-h_{\min 1}}^{h_{\max 1}} e^{[-\frac{(\sigma_1^2 + \sigma_2^2)h_1^2}{2\sigma_1^2 \sigma_2^2} + \frac{h h_1}{\sigma_2^2}] dh_1} . \quad (\text{B.3})$$

Let $\frac{\sigma_1^2 + \sigma_2^2}{2\sigma_1^2 \sigma_2^2} = a_1$, $\frac{h}{\sigma_2^2} = a_2$, then Eq. (B.3) becomes

$$P_h(h) = \frac{1}{2\pi\sigma_1\sigma_2} e^{-h^2/(2\sigma_2^2)} \int_{-h_{\min 1}}^{h_{\max 1}} e^{-a_1 h_1^2 + a_2 h_1} dh_1 = \frac{1}{2\pi\sigma_1\sigma_2} e^{-h^2/(2\sigma_2^2)} \int_{-h_{\min 1}}^{h_{\max 1}} e^{-a_1(h_1 - \frac{a_2}{2a_1})^2 + \frac{a_2^2}{4a_1}} dh_1 = \frac{1}{4\pi\sigma_1\sigma_2} e^{-\frac{h^2}{2\sigma_2^2} + \frac{a_2^2}{4a_1}} \sqrt{\frac{\pi}{a_1}} [\text{erf}(\sqrt{a_1} h_{\max 1} - \frac{a_2}{2\sqrt{a_1}}) - \text{erf}(-\sqrt{a_1} h_{\min 1} - \frac{a_2}{2\sqrt{a_1}})] . \quad (\text{B.4})$$

Wahid and Madhusudana [278] found that the separation between two contacting solid surfaces is about $2.7\sigma_1$, slightly larger than $2.58\sigma_1$ (99% confidence interval of the Gaussian distribution). This might suggest that the effective maximum height of asperity $h_{\max 1}$ and the effective maximum depth of valley, $h_{\min 1}$, could be approximated by $2.7\sigma_1$. If σ_1 is intentionally chosen so that $\sigma_1 \geq \sigma_2$, it would lead to $\sqrt{a_1}h_{\max 1} - \frac{a_2}{2\sqrt{a_1}} \gg 1$, and $-\sqrt{a_1}h_{\min 1} - \frac{a_2}{2\sqrt{a_1}} \ll -1$, which means that $\text{erf}\left(\sqrt{a_1}h_{\max 1} - \frac{a_2}{2\sqrt{a_1}}\right) \sim 1$, and $\text{erf}\left(-\sqrt{a_1}h_{\min 1} - \frac{a_2}{2\sqrt{a_1}}\right) \sim -1$. It would result in $\text{erf}\left(\sqrt{a_1}h_{\max 1} - \frac{a_2}{2\sqrt{a_1}}\right) - \text{erf}\left(-\sqrt{a_1}h_{\min 1} - \frac{a_2}{2\sqrt{a_1}}\right) \approx 2$. Hence, Eq. (B.4) could be approximated as

$$P_h(h) = \frac{1}{2\pi\sigma_1\sigma_2} e^{-\frac{h^2}{2\sigma_2^2} + \frac{a_2^2}{4a_1}} \sqrt{\frac{\pi}{a_1}} = \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} e^{-\frac{h^2}{2(\sigma_1^2 + \sigma_2^2)}}. \quad (\text{B.5})$$

Appendix C. Derivation of the Average Radius of Asperity Curvature, Eq. (7.14)

According to the Majumdar and Bushan (MB) model, the asperity height could be expressed as [217]:

$$h = G'^{D_f-1} l^{2-D_f}, \quad (\text{C.1})$$

where G' is a characteristic length scale determining the position of the spectrum. l is the length scale of a fractal asperity as shown in Figure C.1. The radius of the curvature at the summit of asperity is:

$$R' = \frac{l^{D_f}}{\pi^2 G'^{D_f-1}}. \quad (\text{C.2})$$

The multiplication of Eq. (C.1) and Eq. (C.2) results in:

$$hR' = \frac{l^2}{\pi^2}. \quad (\text{C.3})$$

$h = \sqrt{2}\sigma$ [213]. Generally, there would be approximately equal amount of peaks and valleys [214], which means that $l \approx \frac{\lambda'}{2}$, with λ' the peak to peak distance. Hence, Eq. (C.3) becomes

$$R' \approx \frac{\lambda'^2}{4\sqrt{2}\pi^2\sigma} = \frac{\lambda'^2}{56\sigma}. \quad (\text{C.4})$$

This is in good agreement with the result of Rabinovich et al. [58]: $R' = \frac{\lambda'^2}{58\sigma} = 1.485\sigma$. Therefore, in the proposed model, $R' = 1.485\sigma$ would be used in Eq. (7.6) through Eq. (7.9) to estimate the average approach and deformation.

Figure C.1 A schematic of parameters of asperities

Appendix D. Derivation of the Percentage of Area Covered by Meniscus, Eq. (7.33)

The overall height distribution is resultant by

$$g_h(z) = \int_0^{H_{\max}} g'_h(\zeta) P_h(\zeta - z) d\zeta, \quad (\text{D.1})$$

where $H_{\max}$ is the maximum separation distance available for the formation of meniscus and is equal to R_p for the contact between a spherical particle and a surface.

The deformation of the particle is neglected here for the capillary force calculation, since it is far smaller than $H_{\max}$. Therefore, the percentage of area covered by the meniscus is calculated by the integration of $g_h(z)$ from $-h_{\min}$ to $z - h_{\min}$:

$$G(z) = \int_{-h_{\min}}^{z-h_{\min}} g_h(\zeta) d\zeta, \quad (\text{D.2})$$

where $h_{\min} = h_{\min1} + h_{\min2}$.

The joint probability distribution of surface roughness,

$$P_h(h) = \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} e^{-\frac{h^2}{2(\sigma_1^2 + \sigma_2^2)}}, \quad (\text{D.3})$$

is plugged into Eq. (D.1) for the calculation of the combined height distribution. For a spherical particle of radius R_p on a planar surface, the height distribution of the apparent nominally smooth shape is $g'_h = \frac{2}{R_p^2} (R_p - z)$ [64]. Consequently, Eq. (D.1)

would be

$$g_h(z) = \int_0^{H_{\max}} \frac{2}{R_p^2} (R_p - \zeta) \cdot \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} e^{-\frac{(\zeta-z)^2}{2(\sigma_1^2 + \sigma_2^2)}} d\zeta = \quad (\text{D.4})$$

$$\frac{2}{R_p^2 \sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} \int_0^{H_{\max}} (R_p - \zeta) e^{-\frac{(\zeta-z)^2}{2(\sigma_1^2 + \sigma_2^2)}} d\zeta.$$

Let $\frac{2}{R_p^2 \sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} = B$ and $\sqrt{2(\sigma_1^2 + \sigma_2^2)} = K$, Eq. (D.4) becomes

$$\begin{aligned} g_h(z) &= BR_p \int_0^{H_{\max}} e^{-\frac{(\zeta-z)^2}{K^2}} d\zeta - B \int_0^{H_{\max}} \zeta e^{-\frac{(\zeta-z)^2}{K^2}} d\zeta = \\ &= B(R_p - z)K \left\{ \frac{\sqrt{\pi}}{2} \left[\operatorname{erf}\left(\frac{H_{\max}-z}{K}\right) - \operatorname{erf}\left(-\frac{z}{K}\right) \right] \right\} - \frac{BK^2}{2} \left[e^{-\frac{z^2}{K^2}} - \right. \\ &\quad \left. e^{-\frac{(H_{\max}-z)^2}{K^2}} \right]. \end{aligned} \quad (D.5)$$

Since $H_{\max}$ ($H_{\max} = R_p$) is generally significant larger than z and K which are of the order of magnitude of the effective roughness, it means that $\operatorname{erf}\left(\frac{H_{\max}-z}{K}\right) \sim 1$, and

$e^{-\frac{(H_{\max}-z)^2}{K^2}} \ll e^{-\frac{z^2}{K^2}}$. Therefore, Eq. (D.5) can be simplified to

$$g_h(z) = BR_p K \left\{ \frac{\sqrt{\pi}}{2} \left[1 - \operatorname{erf}\left(-\frac{z}{K}\right) \right] \right\} - \frac{BK^2}{2} e^{-\frac{z^2}{K^2}}. \quad (D.6)$$

Plugging Eq. (D.6) into Eq. (D.2) results in

$$\begin{aligned} G(z) &= \int_{-h_{\min}}^{z-h_{\min}} \{ BR_p K \left\{ \frac{\sqrt{\pi}}{2} \left[1 - \operatorname{erf}\left(-\frac{z}{K}\right) \right] \right\} - \frac{BK^2}{2} e^{-\frac{z^2}{K^2}} \} d\zeta = \\ &= BR_p K \frac{\sqrt{\pi}}{2} \left\{ z - [(z - h_{\min}) \operatorname{erf}\left(-\frac{z-h_{\min}}{K}\right) - \frac{K e^{-\frac{(z-h_{\min})^2}{K^2}}}{\sqrt{\pi}} - \right. \\ &\quad \left. (-h_{\min}) \operatorname{erf}\left(\frac{h_{\min}}{K}\right) + \frac{K e^{-\frac{(h_{\min})^2}{K^2}}}{\sqrt{\pi}}] \right\} - \frac{BK^3}{2} \left[\frac{\sqrt{\pi}}{2} \operatorname{erf}\left(\frac{z-h_{\min}}{K}\right) - \right. \\ &\quad \left. \frac{\sqrt{\pi}}{2} \operatorname{erf}\left(\frac{-h_{\min}}{K}\right) \right]. \end{aligned} \quad (D.7)$$

Putting $B = \frac{2}{R_p^2 \sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}}$ and $K = \sqrt{2(\sigma_1^2 + \sigma_2^2)}$ back into Eq. (D.7) yields

$$G(z) = \quad (D.8)$$

$$\begin{aligned}
& \frac{1}{R_p} \{ z - \\
& [(z - h_{\min}) \operatorname{erf} \left(-\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \\
& \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(z - h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}} - (-h_{\min}) \operatorname{erf} \left(\frac{h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) + \\
& \frac{\sqrt{2(\sigma_1^2 + \sigma_2^2)} e^{-\frac{(h_{\min})^2}{2(\sigma_1^2 + \sigma_2^2)}}}{\sqrt{\pi}}] \} - \frac{\sigma_1^2 + \sigma_2^2}{R_p^2} \left[\operatorname{erf} \left(\frac{z - h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) - \right. \\
& \left. \operatorname{erf} \left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}} \right) \right].
\end{aligned}$$

Appendix E. Comparison of Magnitude of Different Terms in Eq. (7.33)

The analysis was conducted to compare the absolute value of different terms in Eq. (7.33) for the surface roughness of 0.4 – 5 nm and the RH of 30% – 95%, as shown in

Figure E.1. In the figure, A represents $\frac{z}{R_p}$, B represents $\frac{(z-h_{\min})}{R_p} \operatorname{erf}\left(-\frac{z-h_{\min}}{\sqrt{2(\sigma_1^2+\sigma_2^2)}}\right)$, C

represents $\frac{\sqrt{2(\sigma_1^2+\sigma_2^2)} e^{-\frac{(z-h_{\min})^2}{2(\sigma_1^2+\sigma_2^2)}}}{R_p \sqrt{\pi}}$, D represents $\frac{(-h_{\min})}{R_p} \operatorname{erf}\left(\frac{h_{\min}}{\sqrt{2(\sigma_1^2+\sigma_2^2)}}\right)$, E represents

$\frac{\sqrt{2(\sigma_1^2+\sigma_2^2)} e^{-\frac{(h_{\min})^2}{2(\sigma_1^2+\sigma_2^2)}}}{R_p \sqrt{\pi}}$ and F represents $\frac{\sigma_1^2+\sigma_2^2}{R_p^2} \left[\operatorname{erf}\left(\frac{z-h_{\min}}{\sqrt{2(\sigma_1^2+\sigma_2^2)}}\right) - \operatorname{erf}\left(\frac{-h_{\min}}{\sqrt{2(\sigma_1^2+\sigma_2^2)}}\right) \right]$. For

the RH range that satisfies the meniscus formation criterion (Eq. (10.1)) but is not too high (30% < RH < 45%), the magnitude of last term is generally 5 orders of magnitude smaller than other terms. For very high RH (RH > 45%), although the last term might become comparable or even significantly larger than the third term, it is still generally 5 orders of magnitude smaller than the other terms. But the magnitude of the combination of the first five terms is also much larger than the last term, which suggests that the last term could be neglected without major impact to the result.

Figure E.1 The comparison of the magnitude of different terms in Eq. (7.33) in terms of the variation of (a) surface RMS roughness σ_1 ($\sigma_2=0$ nm, RH=40%, $R_p = 2.5$ μ m) and (b) RH ($\sigma_1=0.4$ nm, $\sigma_2=0$ nm).

Appendix F. Comparison of Predictions between Statistical analysis-based Model and Monte Carlo simulation-based Model

The adhesion force distribution for the case of 150 μm PS particles on the stainless steel substrate is predicted by the statistical analysis-based model and Monte Carlo simulation-based model, respectively. The relevant parameters required for modeling are listed in Table 8.1 and Table 8.2. The comparison of the predicted adhesion force distributions is shown by Figure F.1. It is shown that the predicted adhesion force distribution from the statistical analysis-based model is consistent with that from the Monte Carlo simulation-based model.

Figure F.1 The comparison of the predictions between the statistical analysis-based model and the Monte Carlo simulation-based model.

References

1. Corbett, E.L., et al., *The growing burden of tuberculosis: global trends and interactions with the HIV epidemic*. Archives of internal medicine, 2003. **163**(9): p. 1009.
2. Kochi, A., *The global tuberculosis situation and the new control strategy of the World Health Organization*. Bulletin of The World Health Organization, 2001. **79**(1): p. 71-75.
3. Boone, S.A. and C.P. Gerba, *Significance of fomites in the spread of respiratory and enteric viral disease*. Applied and Environmental Microbiology, 2007. **73**(6): p. 1687-1696.
4. Pearson, H., et al., *SARS: what have we learned?* Nature, 2003. **424**(6945): p. 121-126.
5. Radosavljević, V. and B. Jakovljević, *Bioterrorism—Types of epidemics, new epidemiological paradigm and levels of prevention*. Public Health, 2007. **121**(7): p. 549-557.
6. Baillie, L., *The development of new vaccines against Bacillus anthracis*. Journal of Applied Microbiology, 2001. **91**(4): p. 609-613.
7. Kaufmann, A.F., M.I. Meltzer, and G.P. Schmid, *The economic impact of a bioterrorist attack: are prevention and postattack intervention programs justifiable?* Emerging Infectious Diseases, 1997. **3**(2): p. 83.
8. Glover, N.J., *Countering chemical and biological terrorism*. Civil engineering, 2002. **72**(5): p. 62-67.
9. Boone, S.A. and C.P. Gerba, *Significance of fomites in the spread of respiratory and enteric viral disease*. Applied and environmental microbiology, 2007. **73**(6): p. 1687.
10. Kousa, A., et al., *A model for evaluating the population exposure to ambient air pollution in an urban area*. Atmospheric Environment, 2002. **36**(13): p. 2109-2119.
11. Agency, U.E.P., *Air quality criteria for particulate matter*. National Center for Environmental Assessment-RTP Office, 2004.

12. Kowalski, W.J., *Immune building systems technology*. 2003: McGraw Hill Professional.
13. Thatcher, T.L. and D.W. Layton, *Deposition, resuspension, and penetration of particles within a residence*. *Atmospheric Environment*, 1995. **29**(13): p. 1487-1497.
14. Zhou, B., B. Zhao, and Z. Tan, *How Particle Resuspension from Inner Surfaces of Ventilation Ducts Affects Indoor Air Quality—A Modeling Analysis*. *Aerosol Science and Technology*, 2011. **45**(8): p. 996-1009.
15. Ferro, A.R., R.J. Kopperud, and L.M. Hildemann, *Source strengths for indoor human activities that resuspend particulate matter*. *Environmental Science & Technology*, 2004. **38**(6): p. 1759-1764.
16. Ferro, A.R., R.J. Kopperud, and L.M. Hildemann, *Elevated personal exposure to particulate matter from human activities in a residence*. *Journal of Exposure Science and Environmental Epidemiology*, 2004. **14**: p. S34-S40.
17. Qian, J., *Particle resuspension via human activity*. 2007.
18. Qian, J. and A.R. Ferro, *Resuspension of dust particles in a chamber and associated environmental factors*. *Aerosol Science and Technology*, 2008. **42**(7): p. 566-578.
19. Weis, C.P., et al., *Secondary aerosolization of viable Bacillus anthracis spores in a contaminated US Senate Office*. *JAMA: the journal of the American Medical Association*, 2002. **288**(22): p. 2853-2858.
20. Layshock, J.A., et al., *Reaerosolization of Bacillus spp. in Outdoor Environments: A Review of the Experimental Literature*. *Biosecurity and Bioterrorism: Biodefense Strategy, Practice, and Science*, 2012. **10**(3): p. 299-303.
21. Hong, T., et al., *Prioritizing risks and uncertainties from intentional release of selected Category A pathogens*. *PloS one*, 2012. **7**(3): p. e32732.
22. Walter, C.W. and R. Kundsinn, *The floor as a reservoir of hospital infections*. *Surgery, gynecology & obstetrics*, 1960. **111**: p. 412.
23. Kent, D., et al., *Tuberculin conversion. The iceberg of tuberculous pathogenesis*. *Archives of environmental health*, 1967. **14**(4): p. 580.

24. Barker, J. and M. Jones, *The potential spread of infection caused by aerosol contamination of surfaces after flushing a domestic toilet*. Journal of Applied Microbiology, 2005. **99**(2): p. 339-347.
25. Cheesbrough, J., L. Barkess-Jones, and D. Brown, *Possible prolonged environmental survival of small round structured viruses*. The Journal of hospital infection, 1997. **35**(4): p. 325-326.
26. Chen, C., et al., *The effectiveness of an air cleaner in controlling droplet/aerosol particle dispersion emitted from a patient's mouth in the indoor environment of dental clinics*. Journal of The Royal Society Interface, 2010. **7**(48): p. 1105.
27. Goebes, M.D., A.B. Boehm, and L.M. Hildemann, *Contributions of Foot Traffic and Outdoor Concentrations to Indoor Airborne Aspergillus*. Aerosol Science and Technology, 2011. **45**(3): p. 352-363.
28. Price, P.N., et al., *Framework for evaluating anthrax risk in buildings*. Environmental science & technology, 2009. **43**(6): p. 1783-1787.
29. Nazaroff, W.W., *Norovirus, gastroenteritis, and indoor environmental quality*. Indoor air, 2011. **21**(5): p. 353-356.
30. Lai, A.C.K. and W.W. Nazaroff, *Modeling indoor particle deposition from turbulent flow onto smooth surfaces*. Journal of Aerosol Science, 2000. **31**(4): p. 463-476.
31. Sippola, M.R. and W.W. Nazaroff, *Experiments measuring particle deposition from fully developed turbulent flow in ventilation ducts*. Aerosol Science and Technology, 2004. **38**(9): p. 914-925.
32. Krauter, P. and A. Biermann, *Reaerosolization of fluidized spores in ventilation systems*. Applied and environmental microbiology, 2007. **73**(7): p. 2165-2172.
33. Sansone, E.B. and M.W. Slein, *Redispersal of indoor surface contamination: A review*. Journal of Hazardous materials, 1977. **2**(4): p. 347-361.
34. Zuraimi, M., *Is ventilation duct cleaning useful? A review of the scientific evidence*. Indoor Air, 2010. **20**(6): p. 445-457.

35. Thompson, B.P. and L.C. Bank, *Survey of Bioterrorism Risk in Buildings*. Journal of Architectural Engineering, 2008. **14**(1): p. 7-17.
36. Lehtonen, M., T. Reponen, and A. Nevalainen, *Everyday activities and variation of fungal spore concentrations in indoor air*. International Biodeterioration & Biodegradation, 1993. **31**(1): p. 25-39.
37. Crawford, C., et al., *Temporal and spatial variation of indoor and outdoor airborne fungal spores, pollen, and (1 3)- β -D-glucan*. Aerobiologia, 2009. **25**(3): p. 147-158.
38. Buttner, M.P. and L.D. Stetzenbach, *Monitoring airborne fungal spores in an experimental indoor environment to evaluate sampling methods and the effects of human activity on air sampling*. Applied and environmental microbiology, 1993. **59**(1): p. 219-226.
39. Jo, W.K. and Y.J. Seo, *Indoor and outdoor bioaerosol levels at recreation facilities, elementary schools, and homes*. Chemosphere, 2005. **61**(11): p. 1570.
40. Goldmann, D.A., *Transmission of viral respiratory infections in the home*. The Pediatric infectious disease journal, 2000. **19**(10): p. S97.
41. Wan, M., et al., *Modeling the fate of expiratory aerosols and the associated infection risk in an aircraft cabin environment*. Aerosol Science and Technology, 2009. **43**(4): p. 322-343.
42. Nicas, M., *An analytical framework for relating dose, risk, and incidence: an application to occupational tuberculosis infection*. Risk analysis, 1996. **16**(4): p. 527-538.
43. Armstrong, T. and C.N. Haas, *A Quantitative Microbial Risk Assessment Model for Legionnaires' Disease: Animal Model Selection and Dose-Response Modeling*. Risk Analysis, 2007. **27**(6): p. 1581-1596.
44. Armstrong, T.W. and C.N. Haas, *A Quantitative Microbial Risk Assessment Model for Legionnaires' Disease: Animal Model Selection and Dose-Response Modeling*. Risk Analysis, 2007. **27**(6): p. 1581-1596.

45. Atkinson, M.P. and L.M. Wein, *Quantifying the routes of transmission for pandemic influenza*. Bulletin of Mathematical Biology, 2008. **70**(3): p. 820-867.
46. Kowalski, W., W. Bahnfleth, and A. Musser, *Modeling immune building systems for bioterrorism defense*. Journal of Architectural Engineering, 2003. **9**(2): p. 86-96.
47. Reshetin, V.P. and J.L. Regens, *Simulation modeling of anthrax spore dispersion in a bioterrorism incident*. Risk Analysis, 2003. **23**(6): p. 1135-1145.
48. Price, P.N., et al., *Framework for evaluating anthrax risk in buildings*. Environmental Science & Technology, 2009. **43**(6): p. 1783-1787.
49. Hong, T. and P.L. Gurian, *Characterizing Bioaerosol Risk from Environmental Sampling*. Environmental Science & Technology, 2012. **46**(12): p. 6714-6722.
50. Zhou, H., M. Götzinger, and W. Peukert, *The influence of particle charge and roughness on particle–substrate adhesion*. Powder technology, 2003. **135**: p. 82-91.
51. Gady, B., et al., *Identification of electrostatic and van der Waals interaction forces between a micrometer-size sphere and a flat substrate*. Physical Review B, 1996. **53**(12): p. 8065.
52. Bowling, R.A., *An analysis of particle adhesion on semiconductor surfaces*. Journal of the Electrochemical Society, 1985. **132**(9): p. 2208-2214.
53. Bunker, M.J., et al., *Direct observation of single particle electrostatic charging by atomic force microscopy*. Pharmaceutical research, 2007. **24**(6): p. 1165-1169.
54. Johnson, K., K. Kendall, and A. Roberts, *Surface energy and the contact of elastic solids*. Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences, 1971. **324**(1558): p. 301-313.
55. Derjaguin, B., V. Muller, and Y.P. Toporov, *Effect of contact deformations on the adhesion of particles*. Journal of colloid and interface science, 1975. **53**(2): p. 314-326.
56. Rumpf, H., *Die Wissenschaft des Agglomerierens*. Chemie Ingenieur Technik, 1974. **46**(1): p. 1-11.

57. Rabinovich, Y.I., et al., *Adhesion between nanoscale rough surfaces: II. Measurement and comparison with theory*. Journal of colloid and interface science, 2000. **232**(1): p. 17-24.
58. Rabinovich, Y.I., et al., *Adhesion between Nanoscale Rough Surfaces: I. Role of Asperity Geometry*. Journal of colloid and interface science, 2000. **232**(1): p. 10-16.
59. Orr, F., L. Scriven, and A. Rivas, *Pendular rings between solids: meniscus properties and capillary force*. J. Fluid Mech, 1975. **67**(4): p. 723-742.
60. Pakarinen, O., et al., *Towards an accurate description of the capillary force in nanoparticle-surface interactions*. Modelling and Simulation in Materials Science and Engineering, 2005. **13**(7): p. 1175.
61. Beach, E.R. and J. Drelich, *Atomic Force Microscope Pull-off Force Measurements for Insulin in Contact with Acrylonitrile–Butadiene–Styrene and Polypropylene Surfaces at Various Humidities*. Journal of adhesion science and technology, 2011. **25**(4-5): p. 435-449.
62. Çolak, A., et al., *Surface adhesion and its dependence on surface roughness and humidity measured with a flat tip*. Applied surface science, 2012.
63. Rabinovich, Y.I., et al., *Capillary forces between surfaces with nanoscale roughness*. Advances in colloid and interface science, 2002. **96**(1-3): p. 213-230.
64. Butt, H.J., *Capillary forces: Influence of roughness and heterogeneity*. Langmuir, 2008. **24**(9): p. 4715-4721.
65. Greenwood, J. and J. Wu, *Surface roughness and contact: an apology*. Meccanica, 2001. **36**(6): p. 617-630.
66. Robbe-Valloire, F., *Statistical analysis of asperities on a rough surface*. Wear, 2001. **249**(5): p. 401-408.
67. Felicetti, M.A., et al., *Influence of Particle Size, Applied Compression, and Substratum Material on Particle– Surface Adhesion Force Using the Centrifuge Technique*. Industrial & Engineering Chemistry Research, 2008. **48**(2): p. 877-887.

68. Götzinger, M. and W. Peukert, *Particle adhesion force distributions on rough surfaces*. Langmuir, 2004. **20**(13): p. 5298-5303.
69. Lam, K. and J. Newton, *Influence of particle size on the adhesion behaviour of powders, after application of an initial press-on force*. Powder technology, 1992. **73**(2): p. 117-125.
70. Louey, M.D., P. Mulvaney, and P.J. Stewart, *Characterisation of adhesional properties of lactose carriers using atomic force microscopy*. Journal of pharmaceutical and biomedical analysis, 2001. **25**(3-4): p. 559-567.
71. Salazar-Banda, G., et al., *Determination of the adhesion force between particles and a flat surface, using the centrifuge technique*. Powder technology, 2007. **173**(2): p. 107-117.
72. Cooper, K., A. Gupta, and S. Beaudoin, *Simulation of the adhesion of particles to surfaces*. Journal of colloid and interface science, 2001. **234**(2): p. 284-292.
73. Prokopovich, P. and S. Perni, *Multiasperity Contact Adhesion Model for Universal Asperity Height and Radius of Curvature Distributions*. Langmuir, 2010. **26**(22): p. 17028.
74. Prokopovich, P. and S. Perni, *Comparison of JKR-and DMT-based multi-asperity adhesion model: Theory and experiment*. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011. **383**(1): p. 95-101.
75. Williams, J.M., T. Han, and T.P. Beebe Jr, *Determination of single-bond forces from contact force variances in atomic force microscopy*. Langmuir, 1996. **12**(5): p. 1291-1295.
76. Cooper, K., A. Gupta, and S. Beaudoin, *Substrate morphology and particle adhesion in reacting systems*. Journal of Colloid and Interface Science, 2000. **228**(2): p. 213-219.
77. Tsukada, M., et al., *Adhesion force measurement of a DPI size pharmaceutical particle by colloid probe atomic force microscopy*. Powder technology, 2004. **141**(3): p. 262-269.

78. Hinds, W.C., *Aerosol Technology: Properties, Behavior, and Measurement of airborne Particles* (2nd, 1999).
79. Cebeci, T. and A. Smith, *Analysis of Turbulent Boundary Layers*. 1974, Academic Press, New York.
80. Einstein, H.A. and H. Li, *The viscous sublayer along a smooth boundary*. Transactions of the American Society of Civil Engineers, 1958. **123**(1): p. 293-313.
81. Corino, E.R. and R.S. Brodkey, *A visual investigation of the wall region in turbulent flow*. Journal of Fluid Mechanics, 1969. **37**(01): p. 1-30.
82. Smith, C. and S. Schwartz, *Observation of streamwise rotation in the near wall region of a turbulent boundary layer*. Physics of Fluids, 1983. **26**: p. 641.
83. Kline, S., et al., *The structure of turbulent boundary layers*. J. Fluid Mech, 1967. **30**(4): p. 741-773.
84. Kim, H., S. Kline, and W. Reynolds, *The production of turbulence near a smooth wall in a turbulent boundary layer*. J. Fluid Mech, 1971. **50**(1): p. 133–160.
85. Morrison, W., K. Bullock, and R. Kronauer, *Experimental evidence of waves in the sublayer*. Journal of Fluid Mechanics, 1971. **47**(04): p. 639-656.
86. Blackwelder, R. and J. Haritonidis, *Scaling of the bursting frequency in turbulent boundary layers*. Journal of Fluid Mechanics, 1983. **132**(1): p. 87-103.
87. Rao, K.N., R. Narasimha, and M. Narayanan, *The 'bursting' phenomenon in a turbulent boundary layer*. Journal of Fluid Mechanics, 1971. **48**(02): p. 339-352.
88. Luchik, T. and W. Tiederman, *Timescale and structure of ejections and bursts in turbulent channel flows*. Journal of Fluid Mechanics, 1987. **174**(1): p. 529-552.
89. Lu, S. and W. Willmarth, *Measurements of the structure of the Reynolds stress in a turbulent boundary layer*. Journal of Fluid Mechanics, 1973. **60**(3): p. 481-511.
90. Ziskind, G., M. Fichman, and C. Gutfinger, *Resuspension of particulates from surfaces to turbulent flows--Review and analysis*. Journal of aerosol science, 1995. **26**(4): p. 613-644.

91. Alfredsson, P.H., et al., *The fluctuating wall shear stress and the velocity field in the viscous sublayer*. Physics of Fluids, 1988. **31**: p. 1026.
92. Townsend, A., *The properties of equilibrium boundary layers*. Journal of Fluid Mechanics, 1956. **1**(06): p. 561-573.
93. Finnicum, D.S. and T.J. Hanratty, *Turbulent normal velocity fluctuations close to a wall*. Physics of Fluids, 1985. **28**: p. 1654.
94. Kallio, G. and M. Reeks, *A numerical simulation of particle deposition in turbulent boundary layers*. International journal of multiphase flow, 1989. **15**(3): p. 433-446.
95. Leighton, D. and A. Acrivos, *The lift on a small sphere touching a plane in the presence of a simple shear flow*. Zeitschrift für Angewandte Mathematik und Physik (ZAMP), 1985. **36**(1): p. 174-178.
96. Hall, D., *Measurements of the mean force on a particle near a boundary in turbulent flow*. Journal of Fluid Mechanics, 1988. **187**(1): p. 451-466.
97. O'Neill, M., *A sphere in contact with a plane wall in a slow linear shear flow*. Chemical Engineering Science, 1968. **23**(11): p. 1293-1298.
98. Kim, Y., et al., *Source term models for fine particle resuspension from indoor surfaces*. Building and Environment, 2010. **45**(8): p. 1854-1865.
99. Cleaver, J. and B. Yates, *Mechanism of detachment of colloidal particles from a flat substrate in a turbulent flow*. Journal of colloid and interface science, 1973. **44**(3): p. 464-474.
100. Braaten, D., K. Paw U, and R. Shaw, *Particle resuspension in a turbulent boundary layer-observed and modeled*. Journal of aerosol science, 1990. **21**(5): p. 613-628.
101. Matsusaka, S. and H. Masuda, *Particle reentrainment from a fine powder layer in a turbulent air flow*. Aerosol Science and Technology, 1996. **24**(2): p. 69-84.
102. Wen, H. and G. Kasper, *On the kinetics of particle reentrainment from surfaces*. Journal of aerosol science, 1989. **20**(4): p. 483-498.

103. Zhu, Y., et al., *A Particle Resuspension Model in Ventilation Ducts*. Aerosol Science and Technology, 2012. **46**(2): p. 222-235.
104. Giess, P., A. Goddard, and G. Shaw, *Factors affecting particle resuspension from grass swards*. Journal of aerosol science, 1997. **28**(7): p. 1331-1349.
105. Nicholson, K., *Wind tunnel experiments on the resuspension of particulate material*. Atmospheric Environment. Part A. General Topics, 1993. **27**(2): p. 181-188.
106. Goldasteh, I., G. Ahmadi, and A.R. Ferro, *Monte Carlo simulation of micron size spherical particle removal and resuspension from substrate under fluid flows*. Journal of Aerosol Science, 2013. **66**: p. 62-71.
107. Goldasteh, I., G. Ahmadi, and A. Ferro, *A model for removal of compact, rough, irregularly shaped particles from surfaces in turbulent flows*. The Journal of Adhesion, 2012. **88**(9): p. 766-786.
108. Goldasteh, I., G. Ahmadi, and A.R. Ferro, *Wind tunnel study and numerical simulation of dust particle resuspension from indoor surfaces in turbulent flows*. Journal of Adhesion Science and Technology, 2013. **27**(14): p. 1563-1579.
109. Reeks, M., J. Reed, and D. Hall, *On the resuspension of small particles by a turbulent flow*. Journal of Physics D: Applied Physics, 1988. **21**: p. 574.
110. Lazaridis, M., Y. Drossinos, and P.G. Georgopoulos, *Turbulent resuspension of small nondeformable particles*. Journal of colloid and interface science, 1998. **204**(1): p. 24-32.
111. Vainshtein, P., et al., *Kinetic model of particle resuspension by drag force*. Physical review letters, 1997. **78**(3): p. 551-554.
112. Reeks, M. and D. Hall, *Kinetic models for particle resuspension in turbulent flows: theory and measurement*. Journal of aerosol science, 2001. **32**(1): p. 1-31.
113. Anspaugh, L.R., et al., *Movement of radionuclides in terrestrial ecosystems by physical processes*. Health Phys, 2002. **82**(5): p. 669-79.

114. Linsley, G., *Resuspension of the Transuranium Elements: A Review of Existing Data*. 1978: National Radiological Protection Board.
115. Garland, J., *Resuspension of particulate material from grass Experimental programme 1979-1980*. 1982.
116. Loosmore, G.A., *Evaluation and development of models for resuspension of aerosols at short times after deposition*. Atmospheric Environment, 2003. **37**(5): p. 639-647.
117. Oberoi, R., et al., *Human-Induced Particle Re-Suspension in a Room*. Aerosol Science and Technology, 2010. **44**(3): p. 216-229.
118. Corsi, R.L., J.A. Siegel, and C. Chiang, *Particle resuspension during the use of vacuum cleaners on residential carpet*. Journal of Occupational and Environmental Hygiene, 2008. **5**(4): p. 232-238.
119. Qian, J., A.R. Ferro, and K.R. Fowler, *Estimating the resuspension rate and residence time of indoor particles*. Journal of the Air & Waste Management Association, 2008. **58**(4): p. 502-516.
120. Qian, J., J. Peccia, and A.R. Ferro, *Walking-induced particle resuspension in indoor environments*. Atmospheric Environment, 2014. **89**: p. 464-481.
121. Sippola, M.R., R.G. Sextro, and T.L. Thatcher, *Measurements and Modeling of Deposited Particle Transport by Foot Traffic Indoors*. Environmental Science & Technology, 2014. **48**(7): p. 3800-3807.
122. Khalifa, H.E. and B. Elhadidi, *Particle levitation due to a uniformly descending flat object*. Aerosol Science and Technology, 2007. **41**(1): p. 33-42.
123. Kubota, Y., J.W. Hall, and H. Higuchi, *An Experimental Investigation of the Flowfield and Dust Resuspension Due to Idealized Human Walking*. Journal of Fluids Engineering, 2009. **131**: p. 081104.
124. Eisner, A., J. Rosati, and R. Wiener, *Experimental and theoretical investigation of particle-laden airflow under a prosthetic mechanical foot in motion*. Building and Environment, 2010. **45**(4): p. 878-886.

125. Tian, Y., et al., *A comparative study of walking-induced dust resuspension using a consistent test mechanism*. Indoor Air, 2014.
126. Nazaroff, W.W. and G.R. Cass, *Mathematical modeling of indoor aerosol dynamics*. Environmental science & technology, 1989. **23**(2): p. 157-166.
127. Koutrakis, P., S.L.K. Briggs, and B.P. Leaderer, *Source apportionment of indoor aerosols in Suffolk and Onondaga Counties, New York*. Environmental science & technology, 1992. **26**(3): p. 521-527.
128. Schneider, T., J. Kildes, and N. Breum, *A two compartment model for determining the contribution of sources, surface deposition and resuspension to air and surface dust concentration levels in occupied rooms*. Building and Environment, 1999. **34**(5): p. 583-595.
129. Nazaroff, W.W., *Indoor particle dynamics*. Indoor air, 2004. **14**: p. 175-183.
130. Riley, W.J., et al., *Indoor particulate matter of outdoor origin: Importance of size-dependent removal mechanisms*. Environmental Science & Technology, 2002. **36**(2): p. 200-207.
131. McFarland, A., et al., *Aerosol deposition in bends with turbulent flow*. Environmental Science & Technology, 1997. **31**(12): p. 3371-3377.
132. Sippola, M.R. and W.W. Nazaroff, *Modeling particle loss in ventilation ducts*. Atmospheric Environment, 2003. **37**(39): p. 5597-5609.
133. Lai, A.C.K., *Particle deposition indoors: a review*. Indoor Air, 2002. **12**(4): p. 211-214.
134. Long, C.M., et al., *Using time-and size-resolved particulate data to quantify indoor penetration and deposition behavior*. Environmental Science & Technology, 2001. **35**(10): p. 2089-2099.
135. Chan, A.T., *Indoor-outdoor relationships of particulate matter and nitrogen oxides under different outdoor meteorological conditions*. Atmospheric Environment, 2002. **36**(9): p. 1543-1551.

136. Hussein, T., et al., *Particle size characterization and emission rates during indoor activities in a house*. Atmospheric Environment, 2006. **40**(23): p. 4285-4307.
137. Hussein, T., et al., *Emission rates due to indoor activities: Indoor aerosol model development, evaluation, and applications*. Aerosol Science and Technology, 2005. **39**(11): p. 1111-1127.
138. Afshari, A., U. Matson, and L.E. Ekberg, *Characterization of indoor sources of fine and ultrafine particles: a study conducted in a full-scale chamber*. Indoor Air, 2005. **15**(2): p. 141-150.
139. Bagnold, R.A., *The physics of blown sand and desert dunes*. 1941.
140. Braaten, D.A., *Wind tunnel experiments of large particle reentrainment-deposition and development of large particle scaling parameters*. Aerosol Science and Technology, 1994. **21**(2): p. 157-169.
141. Roney, J.A. and B.R. White, *Estimating fugitive dust emission rates using an environmental boundary layer wind tunnel*. Atmospheric Environment, 2006. **40**(40): p. 7668-7685.
142. Rudnick, S. and D. Milton, *Risk of indoor airborne infection transmission estimated from carbon dioxide concentration*. Indoor air, 2003. **13**(3): p. 237-245.
143. Nicas, M., W. Nazaroff, and A. Hubbard, *Toward understanding the risk of secondary airborne infection: emission of respirable pathogens*. Journal of Occupational and Environmental Hygiene, 2005. **2**(3): p. 143-154.
144. Inglesby, T.V., et al., *Anthrax as a biological weapon*. JAMA: the journal of the American Medical Association, 1999. **281**(18): p. 1735-1745.
145. Duguid, J., *The size and the duration of air-carriage of respiratory droplets and droplet-nuclei*. Journal of Hygiene, 1946. **44**(06): p. 471-479.
146. Jennison, M., *Atomizing of Mouth and Nose Secretions into the Air as Revealed by High Speed Photography*, Aerobiology, Washington. Amer. Assoc. for the Advancement of Science, Publication, 1942: p. 106.

147. Loudon, R. and R. Roberts, *Droplet expulsion from the respiratory tract*. The American review of respiratory disease, 1967. **95**(3): p. 435.
148. Papineni, R.A.O.S. and F.S. Rosenthal, *The size distribution of droplets in the exhaled breath of healthy human subjects*. Journal of Aerosol Medicine, 1997. **10**(2): p. 105-116.
149. Chao, C., et al., *Characterization of expiration air jets and droplet size distributions immediately at the mouth opening*. Journal of aerosol science, 2009. **40**(2): p. 122-133.
150. Xie, X., et al., *Exhaled droplets due to talking and coughing*. Journal of The Royal Society Interface, 2009. **6**(Suppl 6): p. S703.
151. Kowalski, W., *Aerobiological engineering handbook*. Aerosol Science and Particle Dynamics. McGraw-Hill, New York, NY, 2006: p. 119.
152. Li, Y., et al., *Role of ventilation in airborne transmission of infectious agents in the built environment—a multidisciplinary systematic review*. Indoor air, 2007. **17**(1): p. 2-18.
153. Kean, T., *The 9/11 commission report: Final report of the national commission on terrorist attacks upon the United States*. Vol. 3. 2011: US Independent Agencies and Commissions.
154. Guha, A., *Transport and deposition of particles in turbulent and laminar flow*. 2008.
155. Lai, A.C., *Particle deposition indoors: a review*. Indoor Air, 2002. **12**(4): p. 211-214.
156. Duizer, E., et al., *Inactivation of caliciviruses*. Applied and environmental microbiology, 2004. **70**(8): p. 4538.
157. Kiseleva, L., *Survival of poliomyelitis, ECHO and Cocksackie viruses in some food products*. Voprosy pitaniia, 1971. **30**(6): p. 58.
158. Brady, M.T., J. Evans, and J. Cuartas, *Survival and disinfection of parainfluenza viruses on environmental surfaces* 1*. American Journal of Infection Control, 1990. **18**(1): p. 18-23.

159. Bean, B., et al., *Survival of influenza viruses on environmental surfaces*. Journal of Infectious Diseases, 1982. **146**(1): p. 47.
160. Ferrier, A., D. Garin, and J. Crance, *Rapid inactivation of vaccinia virus in suspension and dried on surfaces*. Journal of hospital infection, 2004. **57**(1): p. 73-79.
161. Weber, T.P. and N.I. Stilianakis, *Inactivation of influenza A viruses in the environment and modes of transmission: A critical review*. Journal of Infection, 2008. **57**(5): p. 361-373.
162. Sze To, G. and C. Chao, *Review and comparison between the Wells–Riley and dose-response approaches to risk assessment of infectious respiratory diseases*. Indoor Air, 2010. **20**(1): p. 2-16.
163. Yezli, S. and J.A. Otter, *Minimum Infective Dose of the Major Human Respiratory and Enteric Viruses Transmitted Through Food and the Environment*. Food and Environmental Virology: p. 1-30.
164. Tellier, R., *Review of aerosol transmission of influenza A virus*. Emerging Infectious Diseases, 2006. **12**(11): p. 1657-62.
165. Wells, W.F., *Airborne Contagion and Air Hygiene. An Ecological Study of Droplet Infections*. Airborne Contagion and Air Hygiene. An Ecological Study of Droplet Infections., 1955.
166. Nazaroff, W.W., M. Nicas, and S.L. Miller, *Framework for evaluating measures to control nosocomial tuberculosis transmission*. Indoor Air, 1998. **8**(4): p. 205-218.
167. Fisk, W.J., et al., *Economic benefits of an economizer system: energy savings and reduced sick leave*. 2004.
168. Sze To, G. and C. Chao, *Review and comparison between the Wells–Riley and dose response approaches to risk assessment of infectious respiratory diseases*. Indoor air, 2010. **20**(1): p. 2-16.
169. Haas, C.N., J.B. Rose, and C.P. Gerba, *Quantitative microbial risk assessment*. 1999: John Wiley & Sons.

170. Chang, J., K.K. Foarde, and D.W. VanOsdell, *Assessment of fungal (Penicillium chrysogenum) growth on three HVAC duct materials*. Environment International, 1996. **22**(4): p. 425-431.
171. Jiang, H., L. Lu, and K. Sun, *Simulation of particle deposition in ventilation duct with a particle–wall impact model*. Building and Environment, 2010. **45**(5): p. 1184-1191.
172. Wang, S., et al., *An experimental study on short-time particle resuspension from inner surfaces of straight ventilation ducts*. Building and Environment, 2012. **53**: p. 119-127.
173. Sun, K., L. Lu, and H. Jiang, *A numerical study of bend-induced particle deposition in and behind duct bends*. Building and Environment, 2012. **52**: p. 77-87.
174. Klimchitskaya, G., U. Mohideen, and V. Mostepanenko, *Casimir and van der Waals forces between two plates or a sphere (lens) above a plate made of real metals*. Physical Review A, 2000. **61**(6): p. 062107.
175. Al-Malah, K., et al., *Ellipsometric Evaluation of β -Lactoglobulin Adsorption onto Low-and High-Energy Materials*. Biotechnology Progress, 1992. **8**(1): p. 58-66.
176. Israelachvili, J.N., *Intermolecular and surface forces: revised third edition*. 2011: Academic press.
177. Chua, L. and R. Antonia, *The turbulent interaction region of a circular jet*. International communications in heat and mass transfer, 1986. **13**(5): p. 545-558.
178. Roney, J.A. and B.R. White, *Definition and measurement of dust aeolian thresholds*. J. Geophys. Res, 2004. **109**: p. F01013.
179. Lee, S.-R., T.M. Holsen, and S. Dhaniyala, *Design and Development of Novel Large Particle Inlet for PM Larger than 10 μ m (PM₁₀)*. Aerosol Science and Technology, 2008. **42**(2): p. 140-151.
180. Rowe, D.A., et al., *Stride rate recommendations for moderate-intensity walking*. Medicine & Science in Sports & Exercise, 2011. **43**(2): p. 312.
181. Lai, C.Y., et al., *Determination of uniformity of filter deposits*. Aerosol Science and Technology, 2006. **40**(8): p. 607-614.

182. Hall, J.W. and H. Higuchi, *An experimental investigation of the flowfield and dust resuspension due to idealized human walking*. Journal of Fluids Engineering, 2009. **131**: p. 081104-1.
183. Elhadidi, B. and H.E. Khalifa, *Aerodynamic Resuspension of Particles Due to a Falling Flat Disk*. Particulate Science and Technology, 2012(just-accepted).
184. Kubota, Y. and H. Higuchi, *Aerodynamic Particle Resuspension Due to Human Foot and Model Foot Motions*. Aerosol Science and Technology, 2013. **47**(2): p. 208-217.
185. Gillette, D.A., R.E. Lawson, and R.S. Thompson, A "test of concept" comparison of aerodynamic and mechanical resuspension mechanisms for particles deposited on field rye grass (*Secale cercele*). Part 1. Relative particle flux rates. Atmospheric Environment, 2004. **38**(28): p. 4789-4797.
186. Gillette, D.A., R.E. Lawson, and R.S. Thompson, A "test of concept" comparison of aerodynamic and mechanical resuspension mechanisms for particles deposited on field rye grass (*Secale cercele*).—Part 2. Threshold mechanical energies for resuspension particle fluxes. Atmospheric Environment, 2004. **38**(28): p. 4799-4803.
187. Hussein, T., et al., *Deposition rates on smooth surfaces and coagulation of aerosol particles inside a test chamber*. Atmospheric Environment, 2009. **43**(4): p. 905-914.
188. Ayabe, M., et al., *Assessment of minute-by-minute stepping rate of physical activity under free-living conditions in female adults*. Gait & Posture, 2011. **34**(2): p. 292-294.
189. Thio, B.J.R., *Characterization of bioparticulate adhesion to synthetic carpet polymers with atomic force microscopy*. 2008.
190. Mukai, C., J. Siegel, and A. Novoselac, *Impact of airflow characteristics on particle resuspension from indoor surfaces*. Aerosol Science and Technology, 2009. **43**(10): p. 1022-1032.
191. Fromentin, A., *Time dependent particle resuspension from a multi-layer deposit by turbulent flow*. Journal of aerosol science, 1989. **20**(8): p. 911-914.

192. Lamb, R.G. and J.H. Seinfeld, *Mathematical modeling of urban air pollution. General theory*. Environmental Science & Technology, 1973. **7**(3): p. 253-261.
193. Kulmala, M., A. Asmi, and L. Pirjola, *Indoor air aerosol model: the effect of outdoor air, filtration and ventilation on indoor concentrations*. Atmospheric Environment, 1999. **33**(14): p. 2133-2144.
194. Schultz, E., *A comparison of indoor and outdoor particle concentration based on size fractionating deposition measurement*. Journal of Aerosol Science, 1990. **21**: p. S625-S628.
195. Hussein, T., et al., *Indoor and outdoor particle size characterization at a family house in Espoo–Finland*. Atmospheric Environment, 2005. **39**(20): p. 3697-3709.
196. Tippayawong, N., et al., *Indoor/outdoor relationships of size-resolved particle concentrations in naturally ventilated school environments*. Building and Environment, 2009. **44**(1): p. 188-197.
197. Aalto, P., et al., *Aerosol particle number concentration measurements in five European cities using TSI-3022 condensation particle counter over a three-year period during health effects of air pollution on susceptible subpopulations*. Journal of the Air & Waste Management Association, 2005. **55**(8): p. 1064-1076.
198. Vecchi, R., et al., *The role of atmospheric dispersion in the seasonal variation of PM₁ and PM_{2.5} concentration and composition in the urban area of Milan (Italy)*. Atmospheric Environment, 2004. **38**(27): p. 4437-4446.
199. Chen, Q. and L.M. Hildemann, *The effects of human activities on exposure to particulate matter and bioaerosols in residential homes*. Environmental Science & Technology, 2009. **43**(13): p. 4641-4646.
200. Nicas, M. and G. Sun, *An Integrated Model of Infection Risk in a Health-Care Environment*. Risk Analysis, 2006. **26**(4): p. 1085-1096.

201. Schneider, T. and J. Kildes, *A two compartment model for determining the contribution of sources, surface deposition and resuspension to air and surface dust concentration levels in occupied rooms*. Building and Environment, 1999. **34**(5): p. 583-595.
202. Thatcher, T.L., W.A. Fairchild, and W.W. Nazaroff, *Particle deposition from natural convection enclosure flow onto smooth surfaces*. Aerosol Science and Technology, 1996. **25**(4): p. 359-374.
203. Edwards, R.D., E.J. Yurkow, and P.J. Liou, *Seasonal deposition of housedusts onto household surfaces*. Science of the Total Environment, 1998. **224**(1): p. 69-80.
204. USA.com. *Redwood city weather*. 2013; Available from: <http://www.usa.com/redwood-city-ca-weather.htm>.
205. Millage, K.K., et al., *A review of inhalability fraction models: discussion and recommendations*. Inhalation Toxicology, 2010. **22**(2): p. 151-159.
206. Jernigan, J.A., et al., *Bioterrorism-related inhalational anthrax: the first 10 cases reported in the United States*. Emerging Infectious Diseases, 2001. **7**(6): p. 933.
207. Wu, P.C., et al., *Changing microbial concentrations are associated with ventilation performance in Taiwan's air-conditioned office buildings*. Indoor Air, 2005. **15**(1): p. 19-26.
208. Beach, E., et al., *Pull-off force measurements between rough surfaces by atomic force microscopy*. Journal of colloid and interface science, 2002. **247**(1): p. 84-99.
209. Bigerelle, M., T. Mathia, and S. Bouvier, *The multi-scale roughness analyses and modeling of abrasion with the grit size effect on ground surfaces*. Wear, 2012. **286**: p. 124-135.
210. Bora, C., et al., *Multiscale roughness and modeling of MEMS interfaces*. Tribology Letters, 2005. **19**(1): p. 37-48.
211. Archard, J., *Elastic deformation and the laws of friction*. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 1957. **243**(1233): p. 190-205.

212. Ibrahim, A., P. Dunn, and M. Qazi, *Experiments and validation of a model for microparticle detachment from a surface by turbulent air flow*. Journal of aerosol science, 2008. **39**(8): p. 645-656.
213. Persson, B. and E. Tosatti, *The effect of surface roughness on the adhesion of elastic solids*. arXiv preprint cond-mat/0104180, 2001.
214. Persson, B., et al., *On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion*. Journal of Physics: Condensed Matter, 2004. **17**(1): p. R1.
215. Muller, V., V. Yushchenko, and B. Derjaguin, *On the influence of molecular forces on the deformation of an elastic sphere and its sticking to a rigid plane*. Journal of Colloid and Interface Science, 1980. **77**(1): p. 91-101.
216. Greenwood, J. and J. Tripp, *The contact of two nominally flat rough surfaces*. Proceedings of the Institution of Mechanical Engineers, 1970. **185**(1): p. 625-633.
217. Morag, Y. and I. Etsion, *Resolving the contradiction of asperities plastic to elastic mode transition in current contact models of fractal rough surfaces*. Wear, 2007. **262**(5): p. 624-629.
218. Lian, G., C. Thornton, and M.J. Adams, *A theoretical study of the liquid bridge forces between two rigid spherical bodies*. Journal of colloid and interface science, 1993. **161**(1): p. 138-147.
219. Xiao, X. and L. Qian, *Investigation of humidity-dependent capillary force*. Langmuir, 2000. **16**(21): p. 8153-8158.
220. Derjaguin, B.V., *Untersuchungen über die Reibung und Adhäsion, IV*. Colloid & Polymer Science, 1934. **69**(2): p. 155-164.
221. Rabinovich, Y.I., et al., *Measurement of oil-mediated particle adhesion to a silica substrate by atomic force microscopy*. Journal of adhesion science and technology, 2002. **16**(7): p. 887-903.

222. Zhou, H. and W. Peukert, *Modeling adhesion forces between deformable bodies by FEM and hamaker summation*. Langmuir, 2008. **24**(4): p. 1459-1468.
223. Biggs, S. and G. Spinks, *Atomic force microscopy investigation of the adhesion between a single polymer sphere and a flat surface*. Journal of adhesion science and technology, 1998. **12**(5): p. 461-478.
224. Cleaver, J. and L. Looi, *AFM study of adhesion between polystyrene particles;—The influence of relative humidity and applied load*. Powder technology, 2007. **174**(1): p. 34-37.
225. Heim, L.O., et al., *Adhesion forces between individual gold and polystyrene particles*. Journal of adhesion science and technology, 2002. **16**(7): p. 829-843.
226. Krupp, H., *Particle adhesion, theory and experiment*. 1967: Advan. Colloid Interface Sci. 1 (1967), 111-239.
227. Maugis, D. and H. Pollock, *Surface forces, deformation and adherence at metal microcontacts*. Acta Metallurgica, 1984. **32**(9): p. 1323-1334.
228. Quon, R., R. Knarr, and T. Vanderlick, *Measurement of the deformation and adhesion of rough solids in contact*. The Journal of Physical Chemistry B, 1999. **103**(25): p. 5320-5327.
229. Segeren, L., et al., *Microparticle adhesion studies by atomic force microscopy*. Journal of adhesion science and technology, 2002. **16**(7): p. 793-828.
230. Paajanen, M., et al., *Experimental humidity dependency of small particle adhesion on silica and titania*. Journal of colloid and interface science, 2006. **304**(2): p. 518-523.
231. Van Zwol, P., G. Palasantzas, and J.T.M. De Hosson, *Influence of roughness on capillary forces between hydrophilic surfaces*. Physical Review E, 2008. **78**(3): p. 031606.
232. Ata, A., Y.I. Rabinovich, and R.K. Singh, *Role of surface roughness in capillary adhesion*. Journal of adhesion science and technology, 2002. **16**(4): p. 337-346.

233. Matope, S., Y. Rabinovich, and A. Van der Merwe, *Van der Waals interactions between silica spheres and metallic thin films created by e-beam evaporation*. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012.
234. Jacobs, T.D., et al., *The Effect of Atomic-Scale Roughness on the Adhesion of Nanoscale Asperities: A Combined Simulation and Experimental Investigation*. Tribology Letters, 2013: p. 1-13.
235. Leite, F., A. Riul, and P. Herrmann, *Mapping of adhesion forces on soil minerals in air and water by atomic force spectroscopy (AFS)*. Journal of adhesion science and technology, 2003. **17**(16): p. 2141-2156.
236. Tormoen, G.W., J. Drelich, and E.R. Beach, *Analysis of atomic force microscope pull-off forces for gold surfaces portraying nanoscale roughness and specific chemical functionality*. Journal of adhesion science and technology, 2004. **18**(1): p. 1-17.
237. Fukunishi, A. and Y. Mori, *Adhesion force between particles and substrate in a humid atmosphere studied by atomic force microscopy*. Advanced Powder Technology, 2006. **17**(5): p. 567-580.
238. Sedin, D.L. and K.L. Rowlen, *Adhesion forces measured by atomic force microscopy in humid air*. Analytical Chemistry, 2000. **72**(10): p. 2183-2189.
239. Schaefer, D., et al., *Surface roughness and its influence on particle adhesion using atomic force techniques*. Journal of adhesion science and technology, 1995. **9**(8): p. 1049-1062.
240. Coelho, M. and N. Harnby, *Moisture bonding in powders*. Powder technology, 1978. **20**(2): p. 201-205.
241. Houssa, M., et al., *Effect of extreme surface roughness on the electrical characteristics of ultra-thin gate oxides*. Solid-State Electronics, 1999. **43**(1): p. 159-167.
242. Cheng, W., P. Dunn, and R. Brach, *Surface roughness effects on microparticle adhesion*. The Journal of Adhesion, 2002. **78**(11): p. 929-965.

243. Jones, R., et al., *Adhesion forces between glass and silicon surfaces in air studied by AFM: Effects of relative humidity, particle size, roughness, and surface treatment*. Langmuir, 2002. **18**(21): p. 8045-8055.
244. Coelho, M. and N. Harnby, *The effect of humidity on the form of water retention in a powder*. Powder technology, 1978. **20**(2): p. 197-200.
245. Kim, T.-G., et al., *Effects of size, humidity, and aging on particle removal from Si wafers*. Microelectronic Engineering, 2009. **86**(2): p. 145-149.
246. Hsiao, E., M.J. Marino, and S.H. Kim, *Effects of gas adsorption isotherm and liquid contact angle on capillary force for sphere-on-flat and cone-on-flat geometries*. Journal of colloid and interface science, 2010. **352**(2): p. 549-557.
247. De Souza, E., et al., *Capillary forces between chemically different substrates*. Langmuir, 2008. **24**(18): p. 10161-10168.
248. Durst, P.J., et al., *Predicting RMS surface roughness using fractal dimension and PSD parameters*. Journal of Terramechanics, 2011. **48**(2): p. 105-111.
249. Tanaka, M., et al., *Fractal analysis of the influence of surface roughness of toner particles on their flow properties and adhesion behavior*. Powder technology, 2008. **186**(1): p. 1-8.
250. Ergincan, O., G. Palasantzas, and B. Kooi, *Influence of random roughness on cantilever curvature sensitivity*. Applied physics letters, 2010. **96**(4): p. 041912-041912-3.
251. Ferreira, S., et al., *Effect of temperature on the Hurst and growth exponents of CdTe polycrystalline films*. Applied physics letters, 2006. **88**(24): p. 244102-244102-3.
252. Ponson, L., D. Bonamy, and E. Bouchaud, *Two-dimensional scaling properties of experimental fracture surfaces*. Physical review letters, 2006. **96**(3): p. 35506.
253. Zaiser, M., et al., *Self-affine surface morphology of plastically deformed metals*. Physical review letters, 2004. **93**(19): p. 195507.

254. Islam, N., et al., *Surface roughness contribution to the adhesion force distribution of salmeterol xinafoate on lactose carriers by atomic force microscopy*. Journal of Pharmaceutical Sciences, 2005. **94**(7): p. 1500-1511.
255. Eaton, P.J., et al., *Mapping the surface heterogeneity of a polymer blend: an adhesion-force-distribution study using the atomic force microscope*. Langmuir, 2000. **16**(21): p. 7887-7890.
256. Balakrishnan, N. and V.B. Nevzorov, *A primer on statistical distributions*. 2004: Wiley.com.
257. Mott, P., J. Dorgan, and C. Roland, *The bulk modulus and Poisson's ratio of "incompressible" materials*. Journal of Sound and Vibration, 2008. **312**(4): p. 572-575.
258. Owens, D.K. and R. Wendt, *Estimation of the surface free energy of polymers*. Journal of Applied Polymer Science, 1969. **13**(8): p. 1741-1747.
259. Fletcher, M. and G. Loeb, *Influence of substratum characteristics on the attachment of a marine pseudomonad to solid surfaces*. Applied and Environmental Microbiology, 1979. **37**(1): p. 67-72.
260. Ibrahim, A., P. Dunn, and R. Brach, *Microparticle detachment from surfaces exposed to turbulent air flow: Effects of flow and particle deposition characteristics*. Journal of Aerosol Science, 2004. **35**(7): p. 805-821.
261. Cho, E., et al., *Performance of a 1kW-class PEMFC stack using TiN-coated 316 stainless steel bipolar plates*. Journal of Power Sources, 2005. **142**(1): p. 177-183.
262. Sinde, E. and J. Carballo, *Attachment of Salmonella spp. and Listeria monocytogenes to stainless steel, rubber and polytetrafluorethylene: the influence of free energy and the effect of commercial sanitizers*. Food Microbiology, 2000. **17**(4): p. 439-447.
263. Bhattacharya, A. and W. Nix, *Analysis of elastic and plastic deformation associated with indentation testing of thin films on substrates*. International Journal of Solids and Structures, 1988. **24**(12): p. 1287-1298.

264. Hoque, E., et al., *Alkylphosphonate modified aluminum oxide surfaces*. The Journal of Physical Chemistry B, 2006. **110**(22): p. 10855-10861.
265. Zhao, T. and G. Mu, *The adsorption and corrosion inhibition of anion surfactants on aluminium surface in hydrochloric acid*. Corrosion Science, 1999. **41**(10): p. 1937-1944.
266. Good, R.J. and M. Koo, *The effect of drop size on contact angle*. Journal of Colloid and Interface Science, 1979. **71**(2): p. 283-292.
267. Walz, J.Y., L. Suresh, and M. Piech, *The effect of nanoscale roughness on long range interaction forces*. Journal of Nanoparticle Research, 1999. **1**(1): p. 99-113.
268. Herzog Cardoso, A., et al., *Easy polymer latex self-assembly and colloidal crystal formation: the case of poly [styrene-co-(2-hydroxyethyl methacrylate)]*. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1998. **144**(1): p. 207-217.
269. Nguyen, T.T., et al., *A centrifuge method to measure particle cohesion forces to substrate surfaces: The use of a force distribution concept for data interpretation*. International journal of pharmaceutics, 2010. **393**(1): p. 89-96.
270. Giess, P., et al., *Resuspension of monodisperse particles from short grass swards: a wind tunnel study*. Journal of aerosol science, 1994. **25**(5): p. 843-857.
271. Ould-Dada, Z. and N.M. Baghini, *Resuspension of small particles from tree surfaces*. Atmospheric Environment, 2001. **35**(22): p. 3799-3809.
272. You, S. and M.P. Wan, *Mathematical models for the van der Waals force and capillary force between a rough particle and surface*. Langmuir, 2013.
273. Wang, H.C., *Effects of inceptive motion on particle detachment from surfaces*. Aerosol Science and Technology, 1990. **13**(3): p. 386-393.
274. Ibrahim, A., P. Dunn, and R. Brach, *Microparticle detachment from surfaces exposed to turbulent air flow: controlled experiments and modeling*. Journal of aerosol science, 2003. **34**(6): p. 765-782.

- 275. Sharma, M.M., et al., *Factors controlling the hydrodynamic detachment of particles from surfaces*. Journal of colloid and interface science, 1992. **149**(1): p. 121-134.
- 276. Quintanilla, M. and D. Goddard, *Lateral Force Microscopy with micrometer-sized particles: Effect of wear on adhesion and friction*. Wear, 2010. **268**(1): p. 277-286.
- 277. Fuchs, R., et al., *Sliding and rolling of individual micrometre sized glass particles on rough silicon surfaces*. Tribology-Materials, Surfaces & Interfaces, 2013. **7**(2): p. 103-107.
- 278. Wahid, S. and C. Madhusudana, *Gap conductance in contact heat transfer*. International journal of heat and mass transfer, 2000. **43**(24): p. 4483-4487.

Publications

Journal Paper

1. You, S. and Wan, M.P. (2013) Mathematical models for the van der Waals force and capillary force between a rough particle and surface, *Langmuir*.
2. You, S. and Wan, M.P. (2014) Particle concentration dynamics in the ventilation duct after an artificial release: for countering potential bioterrorist attack, *J. Hazard. Mater.*
3. You, S. and Wan, M.P. (2014) Experimental investigation and modeling of human-walking-induced particle resuspension, *Indoor Built Environ.*
4. You, S. and Wan, M.P. (2014) Modeling and experiments of the adhesion force distribution between particles and a surface, *Langmuir*.
5. You, S. and Wan, M.P. (2014) A new turbulent-burst-based model for particle resuspension from rough surfaces in turbulent flow, *Aerosol Science and Technology*. (In press)
6. Modeling the impact of resuspension to infection transmission indoors. (In preparation)

Conference Paper

1. You, S. and Wan, M.P. (2011) Experimental study of particle resuspension from indoor surfaces. *Proceedings of the 12th International Conference on Indoor Air Quality and Climate 2011*.
2. You, S. and Wan, M.P. (2012) A new turbulent burst-based resuspension model with humidity effect, *Proceedings of Healthy Buildings 2012*.

3. You, S. and Wan, M.P. (2014) An Infection Risk Assessment Scheme Incorporating the Effect of Walking-Induced Particle Resuspension. Proceedings of the 13th International Conference on Indoor Air Quality and Climate 2014.