Numerical Modelling of Turbulent Gas-Particle Flow and Its Applications

ZHAOFENG TIAN
B.E., M.E.S

A thesis submitted in fulfilment of the requirement for the degree of
Doctor of Philosophy.

November, 2006

School of Aerospace, Manufacturing & Mechanical Engineering
RMIT University

To the memory of the most admirable and beloved Grandfather Xinglin Du, who has passed away in China while I was carrying out my research in Australia. Thanks to all his guidance, inspiration and encouragement.

Declaration

I, Zhaofeng Tian, hereby submit the thesis titled "*Numerical Modelling of Turbulent gas-particle flow and its Applications*" for the degree of Doctor of Philosophy and certify that the work is my own work except where due acknowledge has been made; the work has not been submitted previously, in whole or in part, for any other academic award; the content of the thesis is the result of work which has been carried out since the official commencement date of the approved research program.

I give consent for this copy of my thesis to be made available for loan and photocopying when handed to the University Library for archiving.

ZHAOFENG TIAN

November 2006

Acknowledgements

First and foremost, I would like to express my deepest gratitude to my supervisor, Professor Jiyuan Tu of the School of Aerospace, Manufacturing & Mechanical Engineering in RMIT University for his fruitful, organised and patient guidance in every aspect of my research work. The immense influence he presented in shaping my research attitude and approach can never be overestimated.

I would also like to express sincere gratitude to my co-supervisor, Dr Guan Heng Yeoh of Australian Nuclear Science and Technology Organization, for the guidance in the Computational Fluid Dynamics and scientific writing.

I would also like to express sincere thanks to Dr William Yang of Commonwealth Scientific and Industrial Research Organization, and Dr Li Chen of Defence Science and Technology Organisation, for their kindly help in developing my knowledge in experimental and numerical approaches.

I would like to thank members of RMIT CFD group and my colleagues in the research office –Dr Hao Tang, Dr Yan Ding, Edsil Dilla, Kiao Inthavong, Dr Shengjin Xu, Dr Rong Situ, Huafeng Li, Dr Randeep Singh, Krishna Mohanarangam, Weng Yew Cheng, Thau Do and Dr Sherman Cheung. They have always provided assistance where necessary.

A special acknowledgement to my family back in China for their care and encouragement throughout my student years, my mother Xiuling Du for her concern and love, my uncle Guowei Du for his constant motivation and support, my sister Zhaoying Tian for her guidance and advice, my wife Jun Chen for her love and encouragement.

Abstract

With the increase of computer power and advancement of modeling software, the study of turbulent gas-particle flow problems using computational fluid dynamics (CFD) techniques is gradually becoming attractive in the engineering field. Two basic CFD approaches are used to simulate the gas-particle flow, i.e. the Eulerian-Lagrangian model and the Eulerian-Eulerian model. The aim of this thesis is three-fold: i) to investigate the performance of both the Eulerian-Lagrangian model and the Eulerian-Eulerian model to simulate the turbulent gas-particle flow; ii) to investigate the indoor airflows and contaminant particle flows using the Eulerian-Lagrangian model; iii) to develop and validate particle-wall collision models and a wall roughness model for the Eulerian-Lagrangian model and to utilize these models to investigate the effects of wall roughness on the particle flows.

In the first part of this thesis, the Eulerian-Lagrangian model in the software package FLUENT (FLUENT Inc.) and the Eulerian-Eulerian model in an in-house research code were employed to simulate the gas-particle flows. The validation against the measurement for two-phase flow over backward facing step and in a 90-degree bend revealed that both CFD approaches provide reasonably good prediction for both the gas and particle phases.

Then, the Eulerian-Lagrangian model was employed to investigate the indoor airflows and contaminant particle concentration in two geometrically different rooms. For the first room configuration, the performances of three turbulence models for simulating indoor airflow were evaluated and validated against the measured air phase velocity data. All the three turbulence models provided good prediction of the air phase velocity, while the Large Eddy Simulation (LES) model base on the Renormalization Group theory (RNG) provided the best agreement with the measurements. As well, the RNG-based LES model is able to provide the instantaneous air velocity and turbulence that are required for the evaluation and design of the ventilation system. In the other two-zone ventilated room configuration, contaminant particle concentration decay within the room was simulated and validated against the experimental data using the RNG-based LES model together with the Lagrangian particle tracking model. The numerical results revealed that the particle-wall

collision model has a considerable effect on the particle concentration prediction in the room.

This research culminates with the development and implementation of particle-wall collision models and a stochastic wall roughness model in the Eulerian-Lagrangian model. This Eulerian-Lagrangian model was therefore used to simulate the gas-particle flow over an in-line tube bank. The numerical predictions showed that the wall roughness has a considerable effect by altering the rebounding behaviours of the large particles and consequently affecting the particles motion downstream along the in-line tube bank and particle impact frequency on the tubes. Also, the results demonstrated that for the large particles the particle phase velocity fluctuations are not influenced by the gas-phase fluctuations, but are predominantly determined by the particle-wall collision. For small particles, the influence of particle-wall collisions on the particle fluctuations can be neglected. Then, the effects of wall roughness on the gas-particle flow in a two-dimensional 90-degree bend were investigated. It was found that the wall roughness considerably altered the rebounding behaviours of particles by significantly reducing the 'particle free zone' and smoothing the particle number density profiles. The particle mean velocities were reduced and the particle fluctuating velocities were increased when taking into consideration the wall roughness, since the wall roughness produced greater randomness in the particle rebound velocities and trajectories.

Work Published During Candidature

During the course of my PhD study, a number of papers have been produced based on the results described in this thesis. Six journal papers have been published or accepted for publication, and another three journal papers have been submitted. Additionally, seven conference papers have been presented in national and international conferences. A detailed publication list is presented below:

Journal papers:

1. **Tian, ZF,** Tu, JY, & Yeoh, GH 2005, 'Numerical simulation and validation of dilute gas-particle flow over a backward-facing step', *Aerosol Science and Technology,* Vol 39, pp. 319-332.

2. **Tian, ZF**, Tu, JY, Yeoh, GH, & Yuen, RKK 2006, 'On the numerical study of contaminant particle concentration in indoor airflow', *Building and Environment,* Vol 41, pp. 1504-1514.

3. Inthavong, K, **Tian, ZF**, Li, HF, Tu, JY, Yang, W, Xue, CL, & Li, CG 2006, 'A numerical study of spray particle deposition in a human nasal cavity', *Aerosol Science and Technology*, Vol 40, pp. 1034-1045.

4. **Tian, ZF**, Tu, JY, & Yeoh, GH 2006, 'Numerical modelling and validation of gas-particle flow in an in-line tube bank', *Computer and Chemical Engineering*, in press.

5. **Tian, ZF**, Tu, JY, & Yeoh, GH 2006, 'CFD studies of indoor airflows and contaminant particle transportations', *Particulate Science and Technology*, in press.

6. **Tian, ZF**, Tu, JY, Yeoh, GH, & Yuen, RKK 2006, 'Numerical studies of indoor airflow and particle dispersion by large eddy simulation', *Building and Environment*, in press.

7. Mohanarangam, K, **Tian, ZF**, & Tu, JY 2006, 'Numerical simulation of Turbulent Gas-Particle Flow in a 90 degree bend: Eulerian approach', submitted.

8. Inthavong, K, **Tian, ZF**, & Tu, JY 2006, 'Optimising nasal spray parameters for efficient drug delivery using CFD', submitted.

9. **Tian, ZF,** Inthavong, K, Tu, JY, & Yeoh, GH 2006, 'Numerical investigation into the effects of wall roughness on a gas-particle flow in a 90-degree bend', submitted.

10. Inthavong, K, **Tian, ZF**, & Tu, JY 2006, 'A numerical study into heat and mass transfer in a human nasal cavity under different inhalation conditions', submitted.

Conference papers:

1. **Tian, ZF**, Tu, JY, Yeoh, GH, & Yuen, RKK 2004, 'Comparison of different *k*-ε models for prediction of transport of particles in a ventilated room', in *Proceedings of 5th International Conference of Multiphase Flow*, Paper number 429, Yokohama, Japan.

2. **Tian, ZF**, Tu, JY, & Yeoh, GH 2004, 'Computational fluid dynamics simulation and validation of dilute gas-particle flow over a backward facing step: Lagrangian versus Eulerian method', in *Proceedings of 3rd International Symposium on Two-phase Flow Modelling and Experimentation*, Paper I-523, Pisa, Italy.

3. **Tian, ZF**, Tu, JY, Yang, W, & Yeoh, GH 2005, 'Numerical simulation and validation of gas-particle flow in a curved duct', in *Proceedings of 5th International Symposium on Multiphase Flow, Heat Mass Transfer and Energy Conversion*, Paper number 213, Xi'An, China.

4. **Tian, ZF**, Tu, JY, & Yeoh, GH 2006, 'Numerical modelling of gas-particle flow over crossflow tube bank', presented in *The 13th Biennial Computational Techniques and Applications Conference*, Townsville, Australia.

5. Mohanarangam, K, **Tian, ZF**, & Tu, JY 2006, 'Numerical simulation of Turbulent Gas-Particle Flow in a 90 degree bend: Eulerian vs. Lagrangian approach', presented in *The 13th Biennial Computational Techniques and Applications Conference*, Townsville, Australia.

6. Li, HF, **Tian, ZF,** Tu, JY, Yang, W, Yeoh, GH, Xue, CL, & Li, CG 2006, 'Studies of airflow through a human nasopharynx and pharynx airway', in *Proceedings of The 5th International Conference on CFD in the Process Industries*, CSIRO, Melbourne, Australia.

7. Inthavong, K, **Tian, ZF**, Li, HF, Tu, JY, Yang, W, Xue, CL, & Li, CG 2006, 'Local deposition sites of drug particles in a human nasal cavity', in *Proceedings of The 5th International Conference on CFD in the Process Industries*, CSIRO, Melbourne, Australia.

Contents

List of Figures

List of Tables

Nomenclature

A_i	convective flux
A_0, A_s	model constants for realizable *k*-*ε* turbulence model
B	diffusion coefficient
B_{gp}, B_ε	model constants for the Eulerian two-fluid model
C_μ	coefficient in the *k*-*ε* turbulence model
C_D	particle drag coefficient
C_{RNG}	constant in RNG LES model
C_1, C_2	model constants for realizable *k*-*ε* turbulence model
$C_{\varepsilon 1}, C_{\varepsilon 2}$	model constants for standard and RNG *k*-*ε* turbulence models
d_p	particle diameter
e	coefficient of restitution
e_n, e_t	mean normal and tangential restitution coefficients
f	correction factor
F_{Di}	aerodynamic drag force
F_{Gi}	gravity force
F_r	Froude number
F_{WMi}	wall-momentum transfer due to particle-wall collision force
g	gravitational acceleration
h	step height
H_r	the mean roughness depth for wall surface

I_{gp}	turbulence interaction between the gas and particle phases for the particle phase turbulent fluctuating energy
l	length scale of energetic turbulent eddies
Lr	the mean cycle of roughness
L_s	characteristic length of the system
Le	eddy length scale
m	ratio of particle to gas density
$\dot{m}$	mass of particles in per unit volume of the gas and particle mixture
P_A^R	the normal impulse due to adhesion during rebound
P_D^A	the normal impulse generated by deformation during approach
P_{kgp}	turbulence production by the mean velocity gradients of two phases
P_k	rate of production term of the turbulent kinetic energy
P_{kp}	production term of the particle fluctuating energy
q_ϕ	general source term
$r*$	normalized radial co-ordinate
r	uniform random number
r_i	radius of curvature of the inner wall (90 degree bend)
r_o	radius of curvature of the outer wall (90 degree bend)
R	strain rate or radius of the 90 degree bend
Re	Reynolds number
R_1	restitution coefficient in the absence of adhesion
S	source term
St	Stokes number
S_{ij}, S_{jk}, S_{ki}	strain rates

t_{cross}	eddy crossing time
t_{int}	eddy-particle interaction time
t_p	particle relaxation time
t_s	system response time
T	fluid temperature
T_L	fluid Lagrangian integral time
u_t^p	particle incident velocity in tangential direction
u_n^p	particle incident velocity in normal direction
u_i, u_j, u_k	velocity
u_o	free stream velocity
V_s	characteristic velocity of the system
v_t^p	particle rebound velocity in tangential direction
v_n^p	particle rebound velocity in normal direction
v_p	particle rebounding velocity
x_i, x_j, x_k	Cartesian coordinate system

Greek letters

α	volume fraction
β	model constant for RNG κ-ε turbulence model
Γ	diffusivity of the scalar
ε	dissipation rate of turbulent kinetic energy
ε_0	the direction of the relative velocity between particle surface and wall

ϕ	governing variable
η	function defined in Equation (6)
η_o	model constant for RNG κ-ε turbulence model
k	turbulent kinetic energy
μ	dynamic viscosity
μ_0	the static friction coefficient
μ_d	dynamic friction coefficient
μ_{eff}	effective turbulent viscosity
μ_t	turbulent viscosity
ν	kinematic viscosity
θ	angle between velocities of the particle and gas
θ	particle incident angle
ρ	density
ρ_1	adhesion coefficient
σ	turbulence Prandtl number
τ_e	eddy life time
τ_f	fluid time scale
τ_ω	wall shear stress
τ_p	particle relaxation time
ω	fluctuating vorticity
ω_p	particle initial angular velocity
ζ	normally distributed random number
Π_{gp}	turbulence interaction between the gas and particle phases for the gas-particle

Ω	vorticity
Ω_p	particle rebounding angular velocity

Subscripts

add	additional
eff	effective
g	gas phase
gp	gas-particle
n	normal direction
p	particle phase
s	solid phase
t	tangential direction or turbulent phase

Superscript

g	gas phase
gp	gas-particle
p	particle phase
ε	dissipation rate of turbulent kinetic energy
κ	turbulent kinetic energy
$(\bar{\ })$	averaged or resolved parameters
$(\ )'$	fluctuation