The copyright of this thesis vests in the author. No quotation from it or information derived from it is to be published without full acknowledgement of the source. The thesis is to be used for private study or non-commercial research purposes only.

Published by the University of Cape Town (UCT) in terms of the non-exclusive license granted to UCT by the author.
Development of a Computationally Efficient Bubble Column Simulation Approach by way of Statistical Bubble Micro-Flow Modelling

Waldo Coetzee

Thesis Presented for the Degree of

DOCTOR OF PHILOSOPHY

in the Department of Chemical Engineering

UNIVERSITY OF CAPE TOWN

March 2013
Abstract

The intimate contact achieved between the gas and liquid phases in bubble columns, coupled with the inherent efficient mixing these reactors offer, yield excellent heat and mass transfer characteristics. These attributes have been exploited commercially for decades, however, due to the complexity of the underlying hydrodynamics, the prediction of bubble columns based on empirical models can be unreliable outside of the operating ranges used to fit these models.

Computational Fluid Dynamics (CFD) has emerged as an attractive tool for simulating these reactors and is based on numerically approximating the fundamentally based Navier-Stokes equations on a discretized domain. The application of CFD has become more practical as the cost of computational resources has declined and has lead to the establishment of three distinct modelling approaches which have been evaluated for the purpose of bubble column simulation in a number of research papers over the past two decades. Here the Euler-Euler approach has been recommended for the simulation of large scale columns, however, this approach is based on the most assumptions and yields the least amount of flow field information. The Euler-Lagrange approach treats bubbles as discrete particles which allows for the incorporation of a deterministic bubble size distribution and the direct consideration of heat and mass transfer effects. The most fundamental approach, Direct Numerical Simulation (DNS), predicts flow properties at the bubble scale, however, is extremely computationally expensive and is therefore only practically applicable to the investigation of a very small number of bubbles.

The objective of this study is to contribute to the simulation of gas-liquid flow interaction occurring in bubble columns by proposing a
novel technique for simulating bubble scale flow information at a significantly reduced computational expense. For this purpose, it is proposed to predict the micro-flow fields around individual bubbles, within an Euler-Lagrange framework, with an algebraic model termed the Bubble Cell Model (BCM). The high gradient regions around individual bubbles are thereby accounted for with an algebraic flow model that can be rapidly evaluated as opposed to the two-phase partial differential Navier-Stokes equations, thereby reducing the numerical complexity of the problem. Since no such flow models currently exist and accuracy and fast evaluation are imperative, a statistical approach to the construction of the BCM is justified.

The construction of the BCM is treated in two stages, where the first stage entails approximating the spatial velocity fields at discrete Reynolds numbers followed by the cross correlation of the stage one models with respect to Reynolds number during the second stage. This is performed such that the resulting model generates the velocity vector field around a bubble for a given Reynolds number (within the operating range).

For the first stage, a Design and Analysis of Computer Experiments (DACE) strategy is investigated, where novel correlation functions and sampling designs are introduced. This approach is shown to be capable of accurately approximating the non-linear velocity fields where the combination of a gradient based sampling strategy and a location dependent correlation function was found to yield the most accurate predictions. In a further investigation, the linear combination of the creeping and potential flow analytical solutions is evaluated and found to accurately predict a significant proportion of the flow field across the operating range, thereby reducing the flow features to be statistically approximated. The residuals from the combined analytical solutions are largely focussed in the wake region for which DACE and empirical modelling strategies are evaluated. The DACE model requires minimal modelling assumptions whereas the empirical
strategy relies on the identification of key features occurring across the operating range and fitting with appropriate models. Both strategies resulted in similar high accuracy approximations with the empirical model requiring fewer parameters and is therefore carried forward to the second stage construction.

The second stage construction involves cross correlating the parameter responses of the stage one model with respect to Reynolds number. This approach is considered reasonable since the flow features develop with the progression of Reynolds number. Smooth responses are obtained when the initial guesses for the stage one fits are used from the previous Reynolds number evaluated. These responses are found to be accurately approximated through a combination of simple exponential and polynomial models, which in conjunction with the stage one model yield the final BCM.

The application of the proposed BCM within an Euler-Lagrange framework is investigated with the adaptation of existing Opensource CFD libraries. A coupling strategy between the BCM and the Eulerian velocity field is proposed which involves the Lagrangian tracking of the bubble centre of mass and the modification of the system of algebraic equations to impose the BCM velocities in the appropriate regions. This strategy is evaluated for the case of a single bubble and for two bubbles rising and compared to the DNS solution obtained using an established implementation of the Volume-Of-Fluid method. The comparison shows the BCM approach capable of accurately simulating bubble scale flow structures at a significantly reduced computational expense, where an approximate order of magnitude decrease in computation time is achieved with the BCM methodology. This positive result highlights the potential of the unique methodology for the simulation of two-phase flow and motivates the extension of the BCM to more operating regimes.
Acknowledgements

I wish to express my gratitude to my supervisor, Assoc. Prof. Randhir Rawatlal, for our frequent discussions that have been an incredible source of ideas and debates that have shaped my thinking over the course of this study. It has been an extremely rich experience that involved endeavours into various aspects of modelling which has been very rewarding. His support has been invaluable.

I would like to thank my co-supervisor, Assoc. Prof. Roelof L. J. Coetzer, for his keen interest in this project and the valuable input he has given. His immense knowledge of statistical science has guided several important aspects of this project. The first seeds of this project was in fact sown in a discussion between my two supervisors prior to my involvement and the upgrade from masters to doctoral level was also made possible through their encouragement, for which I am grateful.

I am very thankful for Prof. Linda M. Haines for our helpful discussions. The process modelling group at the University of Cape Town, members past and present, played a important role through impromptu discussions. To the 4th year students to whom I acted as a co-supervisor, I have learned much from these experiences and I am appreciative to have been able to work with you.

To my girlfriend Anélda, your support has been astonishing and I am grateful for your company throughout this journey. I am also thankful for my parents for their encouragement and support. Finally I would like to thank the sponsor of my studies, Sasol Technology (Pty) Ltd., for making it all possible.
Contents

Abstract i

Contents v

List of Figures ix

List of Tables xv

Nomenclature xxiii

I Background 1

1 Introduction 3

1.1 Fluid dynamics: a brief history ...................... 3

1.2 Computational fluid dynamics ...................... 5

1.3 Bubble columns .................................... 7

1.4 Simulation of bubble columns ....................... 9

1.5 Thesis structure .................................. 11

2 Literature Review 13

2.1 The continuum description .......................... 13

2.2 The Navier-Stokes equations ....................... 15

2.3 Bubble physics ................................... 20

2.3.1 Bubble shape and characteristic parameters ........ 20

2.3.2 Gas-liquid boundary condition .................. 24

2.3.3 Leonardo’s paradox ............................ 27
2.3.4 Transient particle drag ........................................... 29
2.4 Simulation of bubble columns revisited .................................. 31
  2.4.1 Direct numerical simulation ........................................... 32
    2.4.1.1 Moving mesh methods ........................................... 33
    2.4.1.2 Surface tracking methods ........................................ 34
    2.4.1.3 Volume tracking methods ........................................ 35
  2.4.2 Euler-Lagrange ..................................................... 37
  2.4.3 Euler-Euler ....................................................... 39
2.5 The finite volume method ................................................... 41
  2.5.1 Discretisation ....................................................... 41
    2.5.1.1 Time derivative ................................................ 42
    2.5.1.2 Convection ..................................................... 43
    2.5.1.3 Diffusion ....................................................... 43
    2.5.1.4 Source ........................................................ 44
    2.5.1.5 Discretised transport equation ................................ 44
    2.5.1.6 Algebraic equation system ................................... 45
  2.5.2 Solution of the Navier-Stokes equation ............................... 45
2.6 Design and Analysis of Computer Experiments ............................. 47
  2.6.1 Correlation function ............................................... 49
2.7 Critical summary .......................................................... 50

3 Thesis Objectives ............................................................. 51

II Model Development .......................................................... 55

4 Preliminary bubble flow model investigation ................................ 57
  4.1 Bubble Cell Model: Stage one introduction ................................ 58
  4.2 Flow field data generation .............................................. 60
  4.3 Design and Analysis of Computer Experiments ............................. 63
    4.3.1 Correlation function ............................................... 63
    4.3.2 Parameter estimation of correlation functions ...................... 65
  4.4 Sampling Design ........................................................ 66
  4.5 Results and Discussion .................................................. 72
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.5.1</td>
<td>Estimation Criteria</td>
<td>72</td>
</tr>
<tr>
<td>4.5.2</td>
<td>Investigation</td>
<td>74</td>
</tr>
<tr>
<td>4.5.3</td>
<td>Discussion</td>
<td>78</td>
</tr>
<tr>
<td>4.5.3.1</td>
<td>Correlation Function</td>
<td>78</td>
</tr>
<tr>
<td>4.5.3.2</td>
<td>Sampling Designs</td>
<td>79</td>
</tr>
<tr>
<td>4.6</td>
<td>Conclusion</td>
<td>81</td>
</tr>
<tr>
<td>5</td>
<td>Semi-analytical bubble flow model development</td>
<td>83</td>
</tr>
<tr>
<td>5.1</td>
<td>Modelling flow over a fluid sphere</td>
<td>84</td>
</tr>
<tr>
<td>5.1.1</td>
<td>Simplified analytical solutions</td>
<td>84</td>
</tr>
<tr>
<td>5.1.2</td>
<td>General numerical solutions</td>
<td>87</td>
</tr>
<tr>
<td>5.2</td>
<td>Statistical approximations</td>
<td>88</td>
</tr>
<tr>
<td>5.2.1</td>
<td>Combined analytical models</td>
<td>88</td>
</tr>
<tr>
<td>5.2.2</td>
<td>Empirical modelling</td>
<td>91</td>
</tr>
<tr>
<td>5.2.2.1</td>
<td>Fitting of radial velocity residual</td>
<td>91</td>
</tr>
<tr>
<td>5.2.2.2</td>
<td>Fitting of the angular velocity residual</td>
<td>97</td>
</tr>
<tr>
<td>5.2.3</td>
<td>Design and Analysis of Computer Experiments</td>
<td>100</td>
</tr>
<tr>
<td>5.3</td>
<td>Results</td>
<td>104</td>
</tr>
<tr>
<td>5.4</td>
<td>Conclusion</td>
<td>111</td>
</tr>
<tr>
<td>6</td>
<td>Reynolds dependence of semi-analytical flow model</td>
<td>113</td>
</tr>
<tr>
<td>6.1</td>
<td>The Bubble Cell Model stages of construction</td>
<td>114</td>
</tr>
<tr>
<td>6.1.1</td>
<td>Stage one model formulation</td>
<td>114</td>
</tr>
<tr>
<td>6.2</td>
<td>Cross correlation</td>
<td>117</td>
</tr>
<tr>
<td>6.2.1</td>
<td>Sensitivity of the stage one models</td>
<td>117</td>
</tr>
<tr>
<td>6.2.2</td>
<td>Stage two models</td>
<td>119</td>
</tr>
<tr>
<td>6.2.3</td>
<td>Cross validation</td>
<td>121</td>
</tr>
<tr>
<td>6.3</td>
<td>BCM evaluation</td>
<td>123</td>
</tr>
<tr>
<td>6.4</td>
<td>Conclusion</td>
<td>126</td>
</tr>
</tbody>
</table>

III   Model application & Conclusions  129

7   Application of the Bubble Cell Model  131
7.1 Solution procedure .................................................. 132
7.2 Evaluating the BCM ................................................... 134
7.3 Imposing the velocity vector field ................................. 138
7.4 Tracking the BCM centre of mass ............................... 139
7.5 BCM based simulator case study ................................. 140
  7.5.1 Single bubble rising ........................................... 141
  7.5.2 Two bubbles rising ........................................... 143
7.6 Conclusion .......................................................... 151

8 Conclusions .......................................................... 153
  8.1 Future direction ................................................... 155
  8.2 Closure ............................................................ 157

References ............................................................. 159

IV Appendices .......................................................... 177
  A Analytical derivation .............................................. 179
  B Data tables ........................................................ 183
  C Computer code ................................................... 187
List of Figures

1.1 Some of Leonardo’s drawings of flow around obstacles of different geometries (from the Codex Leicester [Leonardo da Vinci, Corbis 1996]). ................................................................. 4

1.2 Schematic of a bubble column: a gas is sparged into a liquid filled vessel and disperses throughout the space resulting in a wide range of time and length scales. In the case of no mechanical mixing, all dispersing energy is introduced via the gas phase. ..................... 8

1.3 The principle flow regimes observed in bubble columns. .............. 9

1.4 A hierarchy of multiphase simulation approaches. ...................... 11

2.1 Approximation through simulation. ........................................ 14

2.2 Concept of pure convection in the principle flow direction. .......... 17

2.3 Random motion of molecules in a stationary liquid causes diffusion across an interface. The same mechanism is responsible for the diffusion of momentum, which involves a fluid with an existing velocity gradient. ................................................. 18

2.4 Schematic of commonly observed bubble shapes. ..................... 22

2.5 Shape regime map for bubbles in liquids (from Bhaga and Weber [1981], see Figure 2.4 for legend). ..................................... 23

2.6 Schematic overview of the effect of contaminants on the gas-liquid interface. From left to right: clean liquid with completely mobile surface corresponding to a zero-shear-stress boundary; slightly contaminated liquid; fully contaminated bubble without any circulation (full no-slip boundary) (adapted from Dijkhuizen et al. [2010]). ................................................................. 26
2.7 The experimentally observed trajectory of a 1.12 mm air bubble in water. (a) Vertical component, (b) $y$ position from camera data, (c) $x$ position from camera data, and (d) three-dimensional reconstruction of full trajectory with greyscale indicating magnitude of acceleration. The bubble begins rising straight, followed by zigzag motion in the $(y,z)$-plane with oscillating velocity, followed by a three-dimensional spiral motion with steady velocity (from Shew et al. [2006]).

2.8 The moving mesh DNS method potentially offers the highest accuracy, however, re-meshing results in significant computational expense.

2.9 Surface markers used for surface tracking methods are used to capture details of the interface on scales smaller than grid spacing.

2.10 The volume fraction distribution function is used to approximate the interface with the volume of fluid volume tracking method.

2.11 Particle tracking of the Euler-Lagrange approach.

2.12 Volume averaging of the Euler-Euler approach.

3.1 The Bubble Cell Model (BCM) concept, the subject of this study.

4.1 The macro model uses the information provided by the BCM to update the flow field around each bubble in the column. The BCM is based on the Navier-Stokes solution of the analogous situation of flow over a sphere which constitutes the BCM experiment.

4.2 Experimental geometry and mesh, the geometry is set up according to the diameter (D) of the bubble and ratio’s chosen to allow flow dynamics to sufficiently develop across the domain.

4.3 Comparison of the simulated drag coefficient with experimental results [Haberman and Morton, 1953] and correlation models [Moore, 1963; Hamielec et al., 1963]

4.4 Distribution of points in the Cartesian space of the UDP with $n_{samp} = 120$.

4.5 Examples of the sampling designs being evaluated.
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6</td>
<td>Scaled $y$-velocity contours for different Reynolds numbers, the blue tones denote higher relative velocities while the red represent the lower flow rates</td>
<td>73</td>
</tr>
<tr>
<td>4.7</td>
<td>Designs and $n_{samp}$ compared based upon the MSE for different surfaces and correlation functions at $Re = 0.1$ and 75</td>
<td>75</td>
</tr>
<tr>
<td>4.8</td>
<td>Designs and $n_{samp}$ compared based upon the MSE for different surfaces and correlation functions at $Re = 270$</td>
<td>76</td>
</tr>
<tr>
<td>4.9</td>
<td>Examples of good fits; marker dots indicate sample points</td>
<td>77</td>
</tr>
<tr>
<td>5.1</td>
<td>Contours of analytical velocity fields. Here $x$ and $y$ denote the Cartesian spatial coordinates centered around the bubble; this is divided by the bubble radius, $R$, for dimensionless coordinates</td>
<td>86</td>
</tr>
<tr>
<td>5.2</td>
<td>Velocity contours for the numerical solution of the axisymmetric Navier-Stokes equations at $Re = 270$</td>
<td>88</td>
</tr>
<tr>
<td>5.3</td>
<td>Cumulative distribution of $u_{r}^{%e}$ and $u_{\theta}^{%e}$</td>
<td>90</td>
</tr>
<tr>
<td>5.4</td>
<td>Residual surface plots at $Re = 135$</td>
<td>92</td>
</tr>
<tr>
<td>5.5</td>
<td>Contours of $</td>
<td>u_{r}^{res}</td>
</tr>
<tr>
<td>5.6</td>
<td>$R^2$ statistic for Eq. 5.17 with respect to radial shells ($r/R$) of $u_{r}^{res}$ at $Re = 270$</td>
<td>95</td>
</tr>
<tr>
<td>5.7</td>
<td>$u_{r}^{m,R1}$ region 1 parameter fitting for $Re = 15$</td>
<td>96</td>
</tr>
<tr>
<td>5.8</td>
<td>$u_{r}^{m,R1}$ region 1 parameter fitting for $Re = 135$</td>
<td>96</td>
</tr>
<tr>
<td>5.9</td>
<td>$u_{r}^{m,R1}$ region 1 parameter fitting for $Re = 270$</td>
<td>97</td>
</tr>
<tr>
<td>5.10</td>
<td>Scaled surface plots of region 2 radial velocity residual ($u_{r}^{res,R2}$) and approximation ($u_{r}^{m,R2}$) at $Re = 270$. The numerical noise in plot (a) is due to very small numerical errors in the CFD simulation</td>
<td>98</td>
</tr>
<tr>
<td>5.11</td>
<td>Contours of $u_{\theta}^{res}/u_{\infty}$ with varying Reynolds number</td>
<td>99</td>
</tr>
<tr>
<td>5.12</td>
<td>Fitting of Eq. 5.22 to $u_{\theta}^{res,R1}$ at $r = R$</td>
<td>100</td>
</tr>
<tr>
<td>5.13</td>
<td>Spatial dependence weighting function $L$ (Eq. 5.32)</td>
<td>103</td>
</tr>
<tr>
<td>5.14</td>
<td>Resulting sample designs, $S$, for $u_{r}^{res}$ at $Re = 270$ with $n_{samp} = 25$</td>
<td>104</td>
</tr>
<tr>
<td>5.15</td>
<td>Comparison of fits using the traditional and proposed Kriging correlation models</td>
<td>106</td>
</tr>
</tbody>
</table>
5.16 Comparison of the best performing DACE fits with the empirical model fits ........................................ 109
5.17 Final residual after Empirical model approximation for $Re = 135$ ........................................ 110
6.1 The two stage BCM fitting strategy ........................................ 115
6.2 Illustration of the critical angle ($\alpha_t^{[17]}$) that divides the domain into two regions, $R_1$ and $R_2$. The contours of the radial velocity residual (i.e., $u_r^t - u_r^{m,a}$) are also depicted ........................................ 116
6.3 Distinct parameters response $\alpha_r^{[10]}$ (Eq. 6.9, $R^2 = 0.9999$). ........................................ 119
6.4 Distinct parameters response $\alpha_r^{[12]}$ (Eq. 6.10, $R^2 = 0.9999$). ........................................ 120
6.5 Distinct parameters response ($\alpha_\theta^{[9]}$ Eq. 6.11, $R^2 = 1.0000$). ........................................ 121
6.6 Distinct parameters response ($\alpha_\theta^{[10]}$ Eq. 6.12, $R^2 = 1.0000$). ........................................ 122
6.7 Scaled velocity vectors of the final BCM evaluated for $Re = 270$ (visualised with ParaView [Ahrens et al., 2005]) ........................................ 124
6.8 $R^2$ statistic of cross correlated radial and angular velocity models ($u_r^M$ and $u_\theta^M$) at different Reynolds numbers on validation data set 126
7.1 The Bubble Cell Model (BCM) concept, the subject of this study. ........................................ 133
7.2 Schematic of the coupling of the BCM within the Navier-Stokes solution procedure ........................................ 134
7.3 Schematic of the BCM evaluation procedure ........................................ 135
7.4 The volume enclosed by the 2-ellipsoidal domain is shown in blue with the volume of the spherical bubble represented by the meshed spherical region ........................................ 136
7.5 Rise velocities of air bubbles in both clean and contaminated water (at 20$^\circ$) for different bubble sizes. The top curve represents the terminal velocity for a clean bubble while the bottom curve corresponds to a contaminated system. The test cases are marked i.e., a clean bubble of 1 mm and 0.9 mm diameter which correspond to terminal velocities of approximately 19 m/s and 18 m/s respectively (from Clift et al. [1978]). ........................................ 142
7.6 A comparison between the rise velocities using the VOF method and the BCM approach for a single bubble test case. The average percentage difference between the velocities is 5.22%. ........................................ 143
7.7 Velocity vector fields for the BCM single bubble test case at three different time steps. ........................................ 144
7.8 Velocity vector fields for the VOF single bubble test case at three different time steps. ........................................ 145
7.9 The experimentally observed wake behind a rectilinear rising air bubble of 1.58 mm diameter in water. On the left the XZ view and on the right the YZ view. (From de Vries [2001]) .................. 146
7.10 A comparison between the rise velocities using the Volume-Of-Fluid method and the BCM approach for the two bubble test case. The average percentage difference between the velocities for the 1 mm bubble is 4.59% and 7.40% for the 0.9 mm bubble. ........ 147
7.11 Bubble trajectories for the two bubble case computed with the VOF and BCM simulators. ................................. 148
7.12 Velocity vector fields for the BCM two bubble test case at three different time steps. ........................................ 149
7.13 Velocity vector fields for the VOF two bubble test case at three different time steps. ........................................ 150
# List of Tables

4.1 Sampling Designs ........................................... 67  
4.2 Comparison of the maximum likelihood (MLE) and residual based parameter estimation criteria ........................................... 74  
4.3 Generation times of DACE models with the EXP, EXP-C and Matérn correlation functions with varying number of sample points, \( n_{samp} \). The times are averaged with respect to the Sampling Design and given in minutes. ........................................... 79  
5.1 Variables with corresponding levels for the DACE model evaluation 105  
5.2 Analysis of Variance for levels of DACE parameters for approximating \( u_r^{\text{res}} \) ........................................... 107  
5.3 Analysis of Variance for levels of DACE parameters for approximating \( u_\theta^{\text{res}} \) ........................................... 107  
5.4 Levels of DACE parameters resulting in lowest MSE for semi-analytical fit ........................................... 108  
5.5 Comparison of the best DACE and empirical semi-analytical solutions for \( u_r \) ........................................... 108  
5.6 Comparison of the best DACE and empirical semi-analytical solutions for \( u_\theta \) ........................................... 108  
6.1 Sensitivities of different stage one models ........................................... 118  
6.2 Summary of second stage models for \( u_r \) ........................................... 122  
6.3 Summary of second stage models for \( u_\theta \) ........................................... 123
7.1 Computational performance of VOF and BCM approaches for 0.1
seconds of simulation time. . . . . . . . . . . . . . . . . . . . . . . . . 147

B.1 Fitting Results for surface Re = 0.1 (results from Chapter 4) . . 183
B.2 Fitting Results for surface Re = 15 (results from Chapter 4) . . . 183
B.3 Fitting Results for surface Re = 75 (results from Chapter 4) . . . 184
B.4 Fitting Results for surface Re = 135 (results from Chapter 4) . . 184
B.5 Fitting Results for surface Re = 270 (results from Chapter 4) . . . 184
B.6 Fitting Results for surface SRD (results from Chapter 4) . . . . . 185
Nomenclature

Roman Symbols

[A] Matrix of coefficients

[R_m] Source vector

ℓ Modified correlation function parameter, local zone function

ˆy Predictor

T Second rank symmetric stress tensor $[Pa]$

A Stage one BCM empirical fitting parameter

B Stage one BCM empirical fitting parameter

C Stage one BCM empirical fitting parameter

d Vector between cell centres $[m]$

F_A Added mass force $[N]$

F_B Buoyancy force $[N]$

F_D Drag force $[N]$

F_G Gravitational force $[N]$

F_H History force $[N]$

f_s Surface force vector field $[Pa]$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>Pressure-velocity coupling operator</td>
<td></td>
</tr>
<tr>
<td>$r$</td>
<td>Radial component</td>
<td>$[m]$</td>
</tr>
<tr>
<td>$S_r$</td>
<td>Surface normal vector</td>
<td>$[m^2]$</td>
</tr>
<tr>
<td>$u_{\phi}^{%e}$</td>
<td>Angular velocity relative error percentage</td>
<td></td>
</tr>
<tr>
<td>$u_{r}^{%e}$</td>
<td>Radial velocity relative error percentage</td>
<td></td>
</tr>
<tr>
<td>$u_{\phi}$</td>
<td>Angular velocity of the creeping flow solution</td>
<td>$[rad/s]$</td>
</tr>
<tr>
<td>$u_{r}$</td>
<td>Radial velocity of the creeping flow solution</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{m,a}$</td>
<td>Linear combination of creeping and potential flow angular velocities</td>
<td>$[rad/s]$</td>
</tr>
<tr>
<td>$u_{r}^{m,a}$</td>
<td>Linear combination of creeping and potential flow radial velocities</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u^m$</td>
<td>Approximate velocity vector field</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{p}$</td>
<td>Angular velocity of the potential flow solution</td>
<td>$[rad/s]$</td>
</tr>
<tr>
<td>$u_{r}^{p}$</td>
<td>Radial velocity of the potential flow solution</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{res}$</td>
<td>Angular velocity residual</td>
<td>$[rad/s]$</td>
</tr>
<tr>
<td>$u_{r}^{res}$</td>
<td>Radial velocity residual</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{t}$</td>
<td>Angular velocity solution obtained numerically</td>
<td>$[rad/s]$</td>
</tr>
<tr>
<td>$u_{r}^{t}$</td>
<td>Radial velocity solution obtained numerically</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u^t$</td>
<td>Numerically obtained velocity vector field</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{r}$</td>
<td>Radial velocity</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\infty}$</td>
<td>Free stream velocity</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{m,R1}$</td>
<td>Angular velocity model in region $R_1$</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{m,R2}$</td>
<td>Angular velocity model in region $R_2$</td>
<td>$[m/s]$</td>
</tr>
<tr>
<td>$u_{\phi}^{res,R1}$</td>
<td>Angular velocity residual in region $R_1$</td>
<td>$[m/s]$</td>
</tr>
</tbody>
</table>
### LIST OF TABLES

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{\theta}^{\text{res},R2}$</td>
<td>Angular velocity residual in region $R_2$</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_{\theta}$</td>
<td>Angular velocity</td>
<td>[rad/s]</td>
</tr>
<tr>
<td>$u_{fs}$</td>
<td>Free stream velocity vector</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_{r}^{m,R1}$</td>
<td>Radial velocity model in region $R_1$</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_{r}^{m,R2}$</td>
<td>Radial velocity model in region $R_2$</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_{r}^{\text{res},R1}$</td>
<td>Radial velocity residual in region $R_1$</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_{r}^{\text{res},R2}$</td>
<td>Radial velocity residual in region $R_2$</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u$</td>
<td>Eulerian velocity vector field</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u^*$</td>
<td>Scaled velocity vector field ($u^* = \frac{u}{</td>
<td></td>
</tr>
<tr>
<td>$v_b$</td>
<td>Bubble velocity vector</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$\mathbb{R}$</td>
<td>Covariance matrix</td>
<td></td>
</tr>
<tr>
<td>$</td>
<td></td>
<td>\cdot</td>
</tr>
<tr>
<td>$a$</td>
<td>Matrix coefficient</td>
<td></td>
</tr>
<tr>
<td>$c$</td>
<td>Linear Kriging weights</td>
<td></td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>Distance function</td>
<td></td>
</tr>
<tr>
<td>$d$</td>
<td>Bubble diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$E[\cdot]$</td>
<td>The expected value operator</td>
<td></td>
</tr>
<tr>
<td>$E_A$</td>
<td>Bubble aspect ratio</td>
<td></td>
</tr>
<tr>
<td>$Eo$</td>
<td>Eötvös number</td>
<td></td>
</tr>
<tr>
<td>$F$</td>
<td>Regression functions evaluated at the sampling points</td>
<td></td>
</tr>
<tr>
<td>$f_i$</td>
<td>Regression function $i$</td>
<td></td>
</tr>
</tbody>
</table>
$f_{s1}$  BCM collective stage one models

$f_{s2}$  BCM collective stage two models

$Fr$  Froude number

$g$  Gravitational acceleration \([m/s^2]\)

$h$  Central difference step size

$i,j$  Mesh point location indices

$K_p$  Modified Bessel function

$Kn$  Knudsen number

$L$  Modified correlation function parameter, combined local zones

$L_{ch}$  Characteristic length \([m]\)

$L_{mol}$  Molecular mean free path \([m]\)

$M$  Morton number

$m$  Desirability function parameter

$m_b$  Bubble mass \([kg]\)

$M_x$  Rotation matrix with respect to x-axis

$M_z$  Rotation matrix with respect to z-axis

$min_d$  Minimum distance parameter

$MSE$  Mean squared error

$n_d$  Number of dimensions

$n_{fscells}$  Number of free stream cells

$n_{grid}$  Number of grid points

$n_{par}$  Number of parameters
**LIST OF TABLES**

- $n_{\text{samp}}$: Number of sample points
- $P$: Eulerian pressure field \([Pa]\)
- $p$: Smoothness parameter
- $P^*$: Scaled pressure field \(P^* = \frac{P-P_{\text{ref}}}{\rho ||\mathbf{v}_b||^r}\)
- $P_{\text{ref}}$: Reference pressure \([Pa]\)
- $R$: Bubble radius \([m]\)
- $r$: Correlation between sample points
- $R_1$: Region 1
- $R_2$: Region 2
- $R_p$: Algebraic equation system source term (excluding pressure)
- $Re$: Reynolds number
- $S$: Sample points
- $s$: Activity of critical point
- $S_\phi$: Source of $\phi$ per unit volume
- $t$: Time \([s]\)
- $u_{\text{rel}}$: Relative bubble velocity
- $V$: Volume \([m^3]\)
- $v$: Specified value for $\phi$
- $V_b$: Bubble volume \([m^3]\)
- $w$: Desirability function parameter
- $We$: Weber number
- $x$: Spatial position
$x_c$  Point of interest
$Y$  Stochastic process
$Y_s$  Sample responses
$Z$  Random process

**Greek Symbols**

$\alpha$  BCM collective stage one model parameters
$\beta_i$  Regression coefficient $i$
$\theta$  Angular component $[rad]$  
$\zeta$  Vorticity $[1/s]$
$\delta^k$  Kronecker delta function
$\delta_{\text{max}}$  Modified correlation function parameter, maximum of local zone
$\delta_{\text{min}}$  Modified correlation function parameter, minimum of local zone
$\delta_R$  Hemi-ellipsoidal weighting factor for $R$
$\delta_{xz}$  Hemi-ellipsoidal weighting factor for $x$ and $z$ direction
$\delta_y$  Top hemi-ellipsoidal weighting factor for $y$
$\eta$  Analytical model weighting coefficient
$\gamma$  BCM collective stage two model parameters
$\Gamma(\cdot)$  Gamma function
$\Gamma_{\phi}$  Diffusion coefficient of $\phi$
$\lambda$  Desirability function dimensional weighting parameter
$\kappa$  Free stream velocity weighting factor
$\mu$  Fluid phase dynamic viscosity $[Pa \cdot s]$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_g$</td>
<td>Gas phase dynamic viscosity</td>
<td>$[Pa \cdot s]$</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Spatial gradient operator</td>
<td>$[1/m]$</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Modified correlation function parameter, local zone slope</td>
<td></td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Velocity potential field</td>
<td>$[m^2/s]$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Tensorial quantity</td>
<td></td>
</tr>
<tr>
<td>$\psi$</td>
<td>Stokes stream function</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>Fluid phase density</td>
<td>$[kg/m^3]$</td>
</tr>
<tr>
<td>$\rho_g$</td>
<td>Gas phase density</td>
<td>$[kg/m^3]$</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>Process variance</td>
<td></td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>Surface tension</td>
<td>$[N/m]$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Shear stress</td>
<td>$[Pa]$</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>Activity of spatial correlation</td>
<td></td>
</tr>
<tr>
<td>$\Theta^*$</td>
<td>Modified activity of spatial correlation</td>
<td></td>
</tr>
<tr>
<td>$\theta_c$</td>
<td>Critical angle</td>
<td>$[rad]$</td>
</tr>
<tr>
<td>$\theta_{a,x}$</td>
<td>BCM rotation angle with respect to $x$-axis</td>
<td>$[rad]$</td>
</tr>
<tr>
<td>$\theta_{a,z}$</td>
<td>BCM rotation angle with respect to $z$-axis</td>
<td>$[rad]$</td>
</tr>
<tr>
<td>$\theta_{mx}$</td>
<td>Rotation w.r.t. $x$-axis of the free stream velocity vector</td>
<td>$[rad]$</td>
</tr>
<tr>
<td>$\theta_{mz}$</td>
<td>Rotation w.r.t. $z$-axis of the free stream velocity vector</td>
<td>$[rad]$</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Stage one BCM empirical fitting parameters</td>
<td></td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Sensitivity of stage one models</td>
<td></td>
</tr>
</tbody>
</table>
Part I

Background
Chapter 1

Introduction

1.1 Fluid dynamics: a brief history

Throughout history mankind has been fascinated by fluid flow and many have sought to describe its underlying physics. The science of fluid dynamics can in fact trace its roots back to the 4th century B.C. when Aristotle established the concept of *continuum* and observed the *resistance* an object experiences when passing through a fluid. He was followed by Archimedes in the 3rd century B.C. who described *static pressure* and the effect of *buoyancy*.

Leonardo da Vinci (1452 - 1519), a keen observer of nature, quantitatively described the *continuity* of incompressible flow through a passage and made sketches of flow around objects, accurately depicting the separation of flow and wake structures (some of these sketches are depicted in Figure 1.1). In addition, Leonardo was intrigued by the motion of air bubbles immersed in water and wrote in one of his notebooks (now known as the Codex Leicester [Leonardo da Vinci, Corbis 1996]):

“The air that is immersed together with the water ... returns to the air by winding its way through the water with a sinuous movement... And this happens because the light thing cannot remain under the heavy”

Leonardo even suggested the modelling of fluid flow through the use of small
Chapter 1. Introduction

finite elements, however, the science of his time was not advanced enough for him to fulfil such a model [Anderson, 2010]. A few centuries later in 1753, Leonard Euler, through the application of Newton’s second law of motion and conservation principles to an infinitesimally small fluid element, was able to derive the partial differential equations for *inviscid flow* (i.e., frictionless flow). These equations represent the beginning of theoretical fluid dynamics and Euler is therefore often cited as the “founder of fluid mechanics” [Tokaty, 1994].

Internal friction was included in 1822 through a complex derivation by Frenchman Claude Louis Marie Henri Navier based on a molecular theory of attraction and repulsion between neighbouring molecules with the viscosity coefficient taken as a function of molecular spacing (this derivation is comprehensively reviewed by Darrigol [2005]). Taking after the work of Navier, another Frenchman Jean Claude Barré de Saint-Venant re-derived the equations in 1843 and correctly identified the coefficient of viscosity and its product with the velocity gradients as viscous stress acting within the fluid due to the influence of friction (unfortunately his name is not associated with these equations). Two years later an Englishman Sir George Gabriel Stokes independently derived the same equations in much the same way they are popularly derived today [Anderson, 2010], that are
now known as the Navier-Stokes equations. The complete mathematical model describing viscous fluid flow has therefore been formulated over 160 years ago.

1.2 Computational fluid dynamics

The Navier-Stokes equations are non-linear, coupled and difficult to solve. Analytical solution is only possible on simple geometries and where the equations have been simplified considerably [Ferziger and Perić, 1999]. The potential of these equations to resolve complex flow phenomenon to address key industrial problems has therefore been largely restricted by the inability to obtain solutions through conventional techniques and explains the delay in their use for many practical problems.

The advent of the computer\(^1\), amongst other achievements, led to the development and increased awareness of the concept of numerical approximation [Hirsch, 2007]. More specifically, the numerical approximation of the Navier-Stokes equations led to the development of a new subset of research in the field of fluid mechanics known as Computational Fluid Dynamics (CFD). The progress in this field has been directly linked to the exponential growth experienced in computing power over the past six decades\(^2\) where the increases in CPU speed, dynamic memory and storage capacity coupled with decreases in costs, have allowed researchers to perform more accurate flow simulations by making fewer simplifications to the flow equations and employ higher resolution grids.

CFD was originally used in the high technology fields of aeronautic, aerospace and naval research. An example of a commercial application is the simulation of flow over an aeroplane at the Airbus company. In 1965 this consisted of solving

\(^1\)The first electronic automatic computer was announced in 1946 and named the ENIAC (Electronic Numerical Integrator And Computer). The development of computing power and its impact is chronicled by Ceruzzi [2003]; Nordhaus [2007].

\(^2\)Increases in computational performance is often associated with the remarkably accurate Moore’s Law, which predicts the number of components on an integrated circuit to increase exponentially. In his original paper [Moore, 1965] predicted doubling of component density every year over a period of ten years, whereafter he modified his prediction to doubling every two years [Moore, 1975].
the potential flow equations over the cross-section of a wing in 2D. Technology
has since progressed to the point, 35 years onwards, of resolving the flow around
a 3D representation of an entire aeroplane using the Navier-Stokes equations,
which has resulted in a significant reduction in the amount of physical prototypes
constructed [Becker, 2002]. The application of CFD has furthermore found its way
into most other aspects of engineering. Notably, CFD in the field of chemical
and process engineering has the potential to yield large savings in equipment
and energy costs and a reduction in environmental pollution [Ferziger and Perić,
1999]. These aspects become increasingly important as tighter legislation and
smaller margins require innovative solutions for commercial operations to remain
competitive.

To counterbalance the benefits CFD has to offer, it should be noted that the nu-
merical solutions are approximate which imparts inherent uncertainty. Potential
error sources include grid skewness, inappropriate numerical schemes and poor
model implementation, and it is therefore advised against using CFD as a black
box modelling tool. Experimental analysis is recommended to be used com-
plimentary to CFD [Versteeg and Malalasekera, 2007]. Furthermore, although
simple problems can be solved using a modern desktop computer within orders
of hours to minutes, complex flow phenomenon e.g., turbulence, compressible
flow and multiphase flow, which often occur simultaneously, can take the order
of weeks to accurately resolve on a cluster of computer processors. Therefore, in
spite of significant increases in hardware capability, computation times have gen-
erally escalated thanks to increases in model complexity in solving the “frontier”
problems [Perić and Bertram, 2011]. In addition, many of these frontier prob-
lems require closure models which are of empirical nature that are the subject of
intense debate.

There remains significant academic and industrial interest in reducing the com-
putation times of CFD simulations. As a conceptual example, consider a 3D
simulation of two-phase flow using a million nodes. Such a case requires the
solution of over nine million non-linear equations at each time step. The size
of the problem further increases when energy and species balances are included.
The exponential growth in computing performance is not guaranteed to continue
indefinitely and certain physical limits exist e.g., the manufacture of transistors at atomic scale, which could prove insurmountable. The present study focuses on one of the frontier problems in CFD, namely, gas-liquid flow occurring in bubble columns and presents the development of a novel technique for simulating bubble scale flow information at a reduced computational expense.

1.3 Bubble columns

Bubble columns are multiphase reactors that involve a dispersed gas phase within a continuous liquid phase (see Figure 1.2). The dispersal of the gas increases the interfacial area whilst the density difference induces relative motion between the phases which results in effective mixing. The high interfacial area together with effective mixing give rise to excellent heat and mass transfer characteristics that coupled with relatively low operating and maintenance costs (stemming from the lack of moving parts) makes bubble columns popular as commercial reactors throughout various industries [Joshi et al., 2002]. Important applications include absorption, desorption, fermentation, Fischer-Tropsch synthesis, flotation and waste water treatment.

The flow in bubble columns can be classified into two principle flow regimes i.e., homogeneous and heterogeneous, which have a significant effect on the operation and performance of these reactors (see Figure 1.3). The homogeneous or bubbly flow regime occurs at low superficial gas velocities, and is characterized by small bubbles of relatively uniform size and rise velocity. Gentle mixing occurs with practically no bubble coalescence or break-up [Kantarci et al., 2005].

At higher superficial gas velocities, the heterogeneous or churn-turbulent regime is prevalent. The heterogeneous regime is characterized by a high variance in the bubble size distribution, ranging from an order of millimeters to centimeters [Matsuura and Fan, 1984]. This flow regime is further complicated by vigorous mixing, frequent bubble coalescence and break-up. The heterogeneous regime is common in commercial scale reactors and presents significant modelling challenges [Kantarci et al., 2005].
Figure 1.2: Schematic of a bubble column: a gas is sparged into a liquid filled vessel and dispenses throughout the space resulting in a wide range of time and length scales. In the case of no mechanical mixing, all dispersing energy is introduced via the gas phase.

Due to considerable industrial interest, the study of bubble columns has attracted a large number of researchers. However, in spite of many publications, the complete understanding of the hydrodynamics has remained elusive. This can be attributed to the complexity of the hydrodynamics of these systems [Kantarci et al., 2005]. The design and scale-up of these reactors has consequently been primarily based on empiricism [Ekambara et al., 2005] which leads to difficulty in scaling up reactor systems from pilot plant studies to industrial scale operations.
Chapter 1. Introduction

1.4 Simulation of bubble columns

CFD has emerged as a promising tool for the simulation of local hydrodynamics in bubble columns and provides detailed flow information that can aid in achieving design objectives. For a reliable design it is desirable to have a detailed knowledge of the flow patterns in bubble columns [Ekambara et al., 2005]. This flow information is very difficult to obtain experimentally and involves expensive apparatus that is often invasive and data that is time consuming to process [Versteeg and Malalasekera, 2007]. In addition, the visualization of the CFD solution data is useful in providing a qualitative understanding of the system.

For the simulation of multiphase systems, three distinct approaches have evolved that can be applied to bubble columns. These are the Direct Numerical Simulation (DNS), Euler-Lagrange and Euler-Euler approaches and will be discussed briefly (these approaches are discussed in more detail in Section 2.4).

The DNS approach is the most fundamentally based and can be used to study very small scale bubble flow detail [Deen et al., 2004]. At its core, DNS entails solving the entire flow field with the Navier-Stokes equations without empirical
Chapter 1. Introduction

closure models. This requires the use of very high resolution grids that, when coupled with the discontinuity of fluid properties across the gas-liquid interface, is extremely computationally expensive to resolve. Convergence of systems with significant differences of fluid properties (such as air and water) can prove difficult. Furthermore, there exist different solution procedures (reviewed in Section 2.4.1) for the treatment of these problems, where no consensus has been reached over their implementation.

The Euler-Lagrange approach usually operates at larger time and length scales, and relies on empirical force models to track individual bubbles in a Lagrangian frame through Newton’s second law of motion. The liquid is treated as a continuum and solved on an Eulerian grid. The discrete nature of the particle treatment allows the dispersed phase properties to be stored and distributions of various properties to be analyzed. This approach is also well suited to the study of bubble-bubble encounters. The computational expense of this approach is proportional to the number of bubbles or particles.

At the largest time and length scales the Euler-Euler (or two fluid) approach is the most suited, although it requires the greatest number of assumptions [Brenner, 2005]. It is usually applied to a single bubble size [Joshi, 2001], but due to its relative computational efficiency for large scale simulations it is currently the best suited approach to industrial scale bubble column simulations.

It follows from the above discussion that the computational expense of simulation increases with the decreasing assumptions and the scale of information required (see Figure 1.4). Delnoij [1999] described these approaches in terms of a “hierarchy of models” where each approach can be used to provide information with respect to different aspects of bubble column operation. It follows that computational expense is an important consideration and a model that can provide high levels of flow detail at a discounted computational expense would be of interest to the multiphase flow community in general.
Chapter 1. *Introduction*

![Figure 1.4: A hierarchy of multiphase simulation approaches.](image)

### 1.5 Thesis structure

This thesis is divided into four primary parts. Part I provides background to the study, which includes this introduction, *Chapter 1*, an examination of the relevant literature, *Chapter 2*, and the thesis objectives, *Chapter 3*. The first two chapters serve to motivate further investigation which is set out in the thesis objectives chapter.

Part II presents the model development, where the development of a micro-flow model around individual bubbles is investigated. *Chapter 4* presents a preliminary investigation, where a Design and Analysis of Computer Experiments (DACE) approach is evaluated for approximating the non-linear velocity fields. *Chapter 5* investigates the use of analytical models together with statistical models to reduce the overall number of parameters. The cross correlation of the model recommended in *Chapter 5* with respect to Reynolds number is evaluated in *Chapter 6*.

The application of the proposed micro-flow model is examined in Part III. The
Chapter 1. *Introduction*

coupling strategy and the resulting simulations are presented in *Chapter 7*. Final conclusions are drawn in *Chapter 8*. The appendices and references are included in Part IV.
Chapter 2

Literature Review

This literature review is concerned with the aspects surrounding the numerical simulation of gas-liquid flows occurring in bubble column reactors. This includes physical and computational aspects of the governing equations, experimental observations and potential statistical models to approximate flow field data. For this purpose, the continuum approximation is examined in Section 2.1, followed by a physical interpretation of the Navier-Stokes equations in Section 2.2. The physics of bubbles is investigated in Section 2.3 with the simulation of bubble columns revisited in Section 2.4. The discretisation of the governing equations with the finite volume method is examined in Section 2.5 and consideration is given to statistical models in Section 2.6. Finally, a critical summary of the literature reviewed is presented in Section 2.7.

2.1 The continuum description

A mathematical model is an abstract of an occurrence in nature, Figure 2.1. The phenomenon of fluid flow is known to be described by a mathematical model, the Navier-Stokes equations, that results from the application of Newton’s second law of motion and conservation principles to an infinitesimal control volume, thereby assuming the fluid to be a continuum. The model is therefore not derived, but
verbally stipulated from the fundamental laws of physics and then formulated as mathematical equations. The validity of these assumptions is inferred from the fact that the resulting description does not conflict with any empirical observation, and is supported by all the available empirical data [Michaelides, 2006].

![Diagram: Approximation through simulation.](image)

Figure 2.1: Approximation through simulation.

It should however be noted that making the continuum assumption assumes a certain scale of reality which is the domain of classical mechanics. At the molecular scale, the fundamental variables are the ones that define the motion of the individual molecules which is of significance for the research of rarefied gasses (e.g., Muntz [1989]). Pressure, temperature, viscosity e.t.c., are mean properties which are deduced from other variables at the basic level of reality [Hirsch, 2007]. Continuum mechanics becomes a valid approximation as the interaction between a high number of particles affects and dominates the motion of each individual particle.

The Knudsen number ($Kn$) can be used to determine whether a material can be treated as a continuum and expresses the ratio of the molecular mean free path ($L_{mol}$) to the characteristic length scale of the system under consideration ($L_{ch}$), see Eq. 2.1. When $Kn$ is near or greater than unity the continuum assumption is no longer a good approximation and statistical methods should be used.

$$Kn = \frac{L_{mol}}{L_{ch}}$$

(2.1)

Given that the order of characteristic dimension of molecules is $10^{-8} \text{ m}$, in the
vast majority of applications involving bubbles, the Knudsen numbers are lower than $10^{-2}$ and, hence, these immersed objects may be approximated as continua [Michaelides, 2006]. It is interesting to note that a continuum assumption can be applied to the study of heavy traffic flow, where the onset of the “fluid mechanical” description is the critical mass where single cars are influenced by the presence of other cars to the extent that the collective motion is superimposed on the individual elements$^1$.

The process of simulation imparts another level of approximation, i.e., the mathematical model itself is approximated through numerical methods (Figure 2.1). Numerical simulation can be prone to errors ranging from insufficient grid resolution, inappropriate discretisation schemes and bad initial conditions. Furthermore, the use of empirical closure models adds uncertainty which could lead to physical approximation error. Given the potential for poor prediction, the physical phenomenon and the physical description of the mathematical model should be considered.

2.2 The Navier-Stokes equations

The history of the Navier-Stokes equations was briefly outlined in Section 1.1. The derivation is not presented in this text as it is reproduced in most fluid dynamics textbooks$^2$. For illustrative purposes, consider the dimensionless form Navier-Stokes equations in vector notation$^3$ (Eq. 2.2 - 2.4).

$^1$The notion of modelling traffic as a continuum was first proposed by renowned fluid mechanics theorist Sir Michael James Lighthill together with applied mathematician Gerald Beresford Whitham [Lighthill and Whitman, 1955]

$^2$A particularly elegant derivation of the Navier-Stokes equations is presented by Ishii and Hibiki [2006]

$^3$The superscripts denotes the scaled quantities
Chapter 2. Literature Review

\[ Re = \frac{\rho d ||v_b||}{\mu} \]  

\[ \nabla^* u^* = 0 \]  

\[ \frac{\partial u^*}{\partial t^*} + (u^* \cdot \nabla^*)u^* = -\nabla^* P^* + \frac{1}{Re} \nabla^2 u^* \]  

In dimensionless form, the influence of the Reynolds number \((Re)\) is explicit and can be interpreted as the relative importance of the inertial forces (convective terms) to the viscous forces (diffusive terms). At very low Reynolds numbers the viscous terms dominate resulting in diffusive behaviour, while with increasing \(Re\), the non-linear convective terms’ influence becomes more pronounced. For high Reynolds numbers it may appear that the viscous terms become entirely negligible, however, they are important in the thin layers adjacent to boundaries, i.e., the boundary layers where velocity gradients are high, and their influence propagates through the rest of the fluid [Clift et al., 1978]. The equations can be classified as parabolic-elliptic [Anderson, 1995], where the combination of the convective and diffusive terms are elliptical in space (i.e., flow can move both forwards and backwards in each spatial direction) while the temporal term is parabolic (i.e., forward marching through time).

The concept of convection is illustrated in Figure 2.2. Here sections of the fluid is signified by tracer particles, which move in the principle flow direction with no velocity gradient in the secondary direction. This scenario can be described by taking the derivative of momentum on a stationary (or Eulerian) grid (Eq. 2.5), which is termed the substantial derivative of momentum [Batchelor, 1967]. Physically, convection is the concerted, collective movement of ensembles of molecules within fluids and the equations describe velocity being convected by velocity with no internal friction within the fluid [Bird et al., 2002].

\[ \rho \frac{Du}{Dt} = \rho \left( \frac{\partial u}{\partial t} + (u \cdot \nabla)u \right) \]  

16
Figure 2.2: Concept of pure convection in the principle flow direction.

For the case of pure diffusion, movement is governed by the random motion of molecules as described by the kinetic theory of gasses (Figure 2.3). This random interaction at the molecular level results in a transfer of momentum which is adequately described for many fluids by Newton’s constitutive shear stress relation (Eq. 2.6). Here the resulting shear stress is linearly proportional to the velocity gradient in the direction perpendicular to the plane of shear and the coefficient of proportionality is termed the dynamic fluid viscosity ($\mu$). The diffusion of momentum can be considered as the internal friction of the fluid. This relation is analogous to the transfer of mass and heat as governed by Fick’s and Fourier’s laws respectively.

$$\tau_{i,j} = \mu \left( \frac{du_i}{dx_j} + \frac{du_j}{dx_i} \right) \quad (i \neq j) \quad (2.6)$$

The stress at an arbitrary point in space is a second rank symmetric tensor ($T$). The fluid pressure corresponds to the mean normal stresses (Eq. 2.7). The surface forces (Eq. 2.10) within the fluid is derived by differentiating the stress tensor over space (Eq. 2.9).
Chapter 2. Literature Review

\[ P = \frac{1}{3} (T_{11} + T_{22} + T_{33}) \]  
\[ T_{ij} = -P \delta_{ij} + \tau_{ij} \]  
\[ f_s = -\nabla P + \nabla \cdot T \]  
\[ f_s = -\nabla P + \mu \nabla^2 u \]

Figure 2.3: Random motion of molecules in a stationary liquid causes diffusion across an interface. The same mechanism is responsible for the diffusion of momentum, which involves a fluid with an existing velocity gradient.

Due to the complex interaction of the convective and diffusive terms, analytical solution of Eq. 2.4 is only possible through simplification. Although the practical relevance of these simplified models is limited, they offer descriptions of fluid flow that are fundamentally based and have therefore been popular for gaining insight into flow problems. The potential flow and creeping flow equations have for these reasons been instrumental in pre-computer fluid dynamics studies.

**Potential flow**

One of the simplest flow models is potential flow (also known as ideal flow) [Ferziger and Perić, 1999]. The fluid is assumed inviscid (effectively eliminating the diffusive terms) and irrotational (Eq. 2.11). Irrotational flow is defined
as flow with zero curl (the curl of the velocity vector is termed vorticity, $\zeta$). This is in contrast to Euler’s equations, where the flow is inviscid without restrictions of the vorticity.

$$\zeta = \nabla \times \mathbf{u} = 0 \quad (2.11)$$

Following from the condition of irrotational flow, there exists a velocity potential ($\Phi$) such that the velocity vector can be defined as the gradient of the potential. Invoking the incompressible continuity equation on this velocity vector, yields a Laplace type equation for $\Phi$ (Eq. 2.12).

$$\nabla \cdot \mathbf{u} = \nabla \cdot (\nabla \Phi) = \nabla^2 \Phi = 0 \quad (2.12)$$

Due to the Laplacian form, potential flow theory results in elegant mathematical solutions and is the subject of many earlier fluid dynamics publications. A major contention however arises from the potential flow prediction of a zero nett force for the flow over a body. This contradiction is described as D’Alembert’s paradox. In contrast, the creeping flow equations can be used to determine a finite drag force.

**Creeping flow**

As the theoretical limit of $Re \to 0$ is approached, the convective terms can be neglected and the flow is termed *creeping flow* which denotes the vanishingly small characteristic velocity of such systems. Under constant fluid properties, the momentum equations become linear and significantly easier to solve. Due to the presence of the viscous terms, these equations carry the ability to enforce the no-slip boundary condition and was famously used to determine the drag over a

---

rigid sphere at low Reynolds numbers by Stokes [1851].

\[
\mu \nabla^2 \mathbf{u} - \frac{1}{\rho} \nabla P = 0 \tag{2.13}
\]

Problems such as the flow over a sphere is solved by writing the creeping flow equations in terms of the Stokes stream function for 2D flows [Slattery, 1999].

### 2.3 Bubble physics

Single bubbles represent the basic elements of a bubble column reactor. Many parallels exist between bubbles, drops and solid particles and therefore modelling strategies for these systems are similar [Clift et al., 1978]. In this context, bubbles are often referred to as fluid particles, which will be used interchangeably throughout this text. Two key distinctions between bubbles and solid particles is the possibility of a bubble to adapt its shape and the different mechanisms between the gas-liquid interface and the solid-liquid interface. These aspects will be discussed in the following subsections.

#### 2.3.1 Bubble shape and characteristic parameters

A bubble assumes the shape that minimizes its total energy [Bozzano and Dente, 2001]. The shape thereby reflects the relative importance of the inertial forces to the surface tension force, which in turn influences the drag experienced. It follows that the velocity and shape of a bubble are strongly coupled. The influence of the shape of a bubble on its rise behaviour was emphasized in the frequently cited paper by Tomiyama et al. [2002]. The researchers also found the method of injection influences the deformation of the bubble shape which in turn has a significant effect on its resulting behaviour in the column. These findings have been confirmed by Wu and Gharib [2002]. The surface tension force drives a bubble towards spherical shape, whereas initial deformation and inertial forces are the primary drivers of non-sphericity.
For gas bubbles rising in liquids, the ratio of the forces exerted by the gas on the interface to the same forces exerted by the liquid on the interface are $\rho_g/\rho$ and $\mu_g/\mu$, which are in the order of $10^{-3}$ and $10^{-2}$ respectively\textsuperscript{1} [Harper and Moore, 1968; Bhaga, 1976]. The amount of variables can therefore be reduced through the assumption that the enclosed gas has a negligible effect on the flow. The remaining variables characterising the system can be combined in a series of dimensionless numbers which is useful for summarising system properties (Eq. 2.2, 2.14 - 2.17). These numbers are termed the Reynolds, Eötvös, Morton, Weber, Froude numbers respectively. $C_D$ is referred to as the drag coefficient.

$$Re = \frac{\rho d ||v_b||}{\mu} \propto \frac{\text{inertial force}}{\text{viscous force}}$$ (2.2)

$$Eo = \frac{g(\rho - \rho_g)d^2}{\sigma_s} \propto \frac{\text{buoyancy force}}{\text{surface tension force}}$$ (2.14)

$$M = \frac{g\mu^4(\rho - \rho_g)}{\rho^2\sigma_s^3} = \text{liquid properties}$$ (2.15)

$$We = \frac{\rho ||v_b||^2d}{\sigma_s} \propto \frac{\text{inertial force}}{\text{surface tension force}}$$ (2.16)

$$Fr = \frac{||v_b||^2}{gd} \propto \frac{\text{buoyancy force}}{\text{inertial force}}$$ (2.17)

$$C_D = \frac{4gd}{3||v_b||^2} \propto \frac{\text{buoyancy force}}{\text{inertial force}}$$ (2.18)

Many of the variables are repeated in these dimensionless numbers and they are not all independent. In fact only three of these groups are independent, which can be used to describe the characteristics of a bubble [Bhaga, 1976]. Grace [1973] correlated the data for 21 different liquids with disparate physical properties to the Reynolds, Eötvös and Morton numbers. He identified that bubble shapes can be classified into three distinct shape regimes i.e., spherical, ellipsoidal and spherical-cap. Bhaga and Weber [1981] extended the correlation to include detailed variations of the shape regimes i.e., oblate ellipsoidal-cap, wobbling disc-like oblate ellipsoidal, skirted bubbles with smooth steady laminar skirts, skirted

\textsuperscript{1}For an air water system at 20°C: $\rho_g/\rho = 1.21 \cdot 10^{-3}$ and $\mu_g/\mu = 1.82 \cdot 10^{-2}$
Chapter 2. Literature Review

bubbles with wavy unsteady skirts, spherical-cap with closed toroidal wake and spherical-cap with open unsteady wake (see Figure 2.4 and 2.5). Loth [2008] proposed various models correlating the bubble aspect ratio ($E_a$, i.e., the ratio of the major and minor axis of a bubble) to $We$ based on the experimental investigations of other researchers, illustrating how bubble shape can be parameterized. The three major bubble shape groups are outlined in the paragraphs below.

![Bubble Shapes Diagram]

Figure 2.4: Schematic of commonly observed bubble shapes.

**Spherical bubbles**

For spherical bubbles, the surface tension force which tends to minimize the surface area of the fluid particle, dominates the inertial forces. This occurs at either sufficiently low Reynolds or Eötvös numbers as evident from Figure 2.5. Saito [1913] showed that in the creeping flow limit a fluid particle of any viscosity
Figure 2.5: Shape regime map for bubbles in liquids (from Bhaga and Weber [1981], see Figure 2.4 for legend).
ratio and \( \text{We} \) or \( Eo \) will remain spherical. For an air-water system, this regime occurs at \( Eo < 0.14 \) or \( Re < 270 \) [Clift et al., 1978].

**Ellipsoidal bubbles**

Ellipsoidal bubbles are found at relatively high Reynolds number and intermediate Eötvös number. Due to the nature of the pressure field (i.e., high pressure at the front and low pressure at the sides following from Bernoulli’s principle) the shape tends toward oblate rather than prolate (i.e., \( E_a < 1 \)). Loth [2008] defined a bubble as ellipsoidal when \( E_a < 0.9 \). These bubbles commonly undergo periodic dilations or random wobbling motions which make characterization of the shape difficult [Bhaga, 1976]. For an air-water system, ellipsoidal bubbles occur at \( 0.14 < Eo < 0.14 \) or \( 270 < Re < 4700 \) [Clift et al., 1978].

**Spherical-cap bubbles**

Spherical-cap bubbles are defined as all bubbles with flat or indented bases without fore and aft symmetry. These bubbles look similar to segments cut from spheres or from ellipsoids. Spherical-cap bubbles in highly viscous liquids have in some cases been reported to trail very thin sheets of gas referred to as “skirts” [Harper, 1970], as shown in the spherical-cap regime on Figure 2.5. The aspect ratio for a spherical-cap bubble is defined as less than 0.25 [Loth, 2008]. For an air-water system, dimensionless parameters correspond to \( Eo > 40 \) or \( Re > 4700 \) [Clift et al., 1978].

### 2.3.2 Gas-liquid boundary condition

The independent studies by Hadamard [1911] and Rybczynski [1911] are often cited as the starting point to bubble motion research. By solving the creeping flow equation for the flow over a spherical fluid particle, and assuming continuity of tangential velocity across the interface, they determined the drag coefficient to be equal to \( 2/3 \) of a rigid body with otherwise identical properties (computed using...
Stokes’ law). This results in a prediction of terminal velocities up to 50% higher than the corresponding rigid particles, however, it is experimentally observed that small bubbles follow Stokes law rather than the Hadamard-Rybczynski theory. Several explanations followed (e.g., Bond and Newton [1928]), however, it was the surface contamination theory proposed by Frumkin and Levich [1947] that was found to sufficiently describe this phenomena. It follows that surface-active contaminants which are present in the liquid phase tend to accumulate at the gas-liquid interface and are swept to the rear of the bubble. The arising concentration gradient at the interface results in a tangential gradient of surface tension which in turn causes a tangential stress tending to retard surface motion.

These findings led to the conclusion that a fully contaminated system results in bubbles with immovable interfaces which can effectively be treated as rigid particles i.e., a no-slip boundary condition is appropriate [Loth, 2008]. For a clean system, the boundary condition corresponds to a zero-shear-stress treatment as used by Hadamard-Rybczynski [Batchelor, 1967; Magnaudet and Eames, 2000]. In between these two extrema, the surface tension gradient can be modelled and is referred to as the Marangoni effect [Tuković and Jasak, 2012]. The Marangoni effect can also arise due to a temperature gradient along the interface [Michaelides, 2006].

The zero-shear-stress boundary condition causes the fluid to slip along the interface in contrast to sticking to it as is the case with the no-slip condition, very often making the flow unseparated in cases where flow around a rigid object of similar shape would be separated or even turbulent [Magnaudet and Eames, 2000]. This change in the separation point affects the shape of the flow field and is an important consideration when the momentum, concentration and thermal boundary layers are investigated. The influence of the surface condition can be observed by way of the terminal velocity of air bubbles in water across the Reynolds number range [Gaudin, 1957]. Here the difference in terminal velocities for clean and contaminated systems are significant for spherical and ellipsoidal bubbles, while spherical-cap bubbles experience a negligible influence.

With the effect of surface-active contaminants established it should furthermore be noted that gas-liquid systems are highly susceptible to their presence. Water
commonly used in experiments is often classified as tap water, distilled water or hyper-clean water [Loth, 2008]. Distilled water is obtained by heating water to form vapour which leaves behind impurities that have higher boiling points, however, many organic substances have similar or lower boiling points, which makes them difficult to remove via distillation. To further purify the water, various filtration systems and UV light are employed to remove surfactants which is then classified as hyper-clean water.

Figure 2.6: Schematic overview of the effect of contaminants on the gas-liquid interface. From left to right: clean liquid with completely mobile surface corresponding to a zero-shear-stress boundary; slightly contaminated liquid; fully contaminated bubble without any circulation (full no-slip boundary) (adapted from Dijkhuizen et al. [2010]).

The use of the Navier-Stokes equations to simulate the flow over a single bubble was considered by McMahon [2009] in a precursor to the present study. Due to the lack of appropriate experimental results (because of the difficulty in non-invasive quantitative measurements of the micro-flow field around an individual bubble), the flow over a rigid sphere was considered for which experimental results is available. Good qualitative agreement in the general flow structure and close quantitative agreement in the non-dimensionless wake length was found in
the Reynolds number range considered (i.e., $Re$ from 26.8 - 90). McMahon [2009] argued that since the gradients for a zero-shear-stress boundary condition (appropriate for a bubble) is not as sharp as for a no-slip boundary condition, the numerical results for the zero-shear-stress case can be accepted as sufficiently accurate.

### 2.3.3 Leonardo’s paradox

Theoretically it could be expected that a single axisymmetric bubble rising in a stagnant liquid would follow a rectilinear path (i.e., rise in a straight path). This is indeed observed experimentally for small spherical and larger spherical-cap bubbles, however, for bubbles in between these extremes, either a zigzag (rocking) or helical trajectory is observed (e.g., Ellingsen and Risso [2001]; de Vries et al. [2002]; Brenn et al. [2006]). Shew et al. [2006] observed through the use of ultrasound and a high-speed video camera that a bubble typically starts out on a straight path from where it transitions to a zigzag trajectory and eventually, for a long enough column, enters into a stable helical motion (see Figure 2.7). Prosperetti [2004] termed this phenomenon of non-rectilinear bubble trajectory “Leonardo’s paradox” paying homage to Leonardo’s meticulous observations. The physics of Leonardo’s time held the view that every movement preserves the course from its inception, which was clearly contradicted by the motion of a rising bubble [Prosperetti, 2004].

It has been suggested that the origin of non-rectilinear motion is due to vortex shedding at the rear of the bubble [Brücker, 1999]. This view has been superseded by the explanation that the lateral force stems from the development of a two-threaded bubble wake with opposite circulation, arising when the bubble is large enough to deform into an ellipsoid. It was observed by de Vries et al. [2002] that the double-threads are present whenever the curvature of the bubble path is non-zero and a single thread occurs when the curvature of the path is zero. The occurrence of the double-threads result in a lateral force directed to the centre of the curvature path which results in the oscillating motion.

As a bubble rises in a stagnant liquid it is observed that the minor axis is approx-
Chapter 2. Literature Review

Force measurements on rising bubbles

Figure 2. Example trajectory of a 1.12 mm radius bubble (at 1 atm). (a) Vertical component of velocity as measured with ultrasound technique, (b) y position from camera data, (c) x position from camera data, and (d) three-dimensional reconstruction of full trajectory with greyscale indicating magnitude of acceleration. The bubble begins rising straight, followed by zigzag motion in the (y,z)-plane with oscillating velocity, followed by a three-dimensional spiral motion with steady velocity (from Shew et al. [2006]).

Figure 3. (a) Projection of a bubble trajectory onto a horizontal plane during the transition from zigzag to spiral (see also x and y data in figures 2(b) and 2(c)). Greyscale indicates time: black at $t=0$ and light grey at $t=4$ s. The bubble radius is 1.12 mm at 1 atm. (b) Diagram of the coordinate system, velocity $U$, pitch angle $\theta$, and external forces ($F_B$, $F_D$, $F_L$) present for a spiralling bubble. The dashed lines lie in the $1-2$ plane.
Chapter 2. Literature Review

approximately aligned with the bubble path [Ellingsen and Risso, 2001; de Vries et al., 2002; Veldhuis et al., 2008]. Ellingsen and Risso [2001]; Shew et al. [2006] found the shape of a rising bubble to be steady, while de Vries et al. [2002] observed slight shape oscillations during zigzag motion and steady shape during helical motion. Loth [2008] noted that the shape of a bubble “adapts almost immediately to local flow conditions”, which justifies the use of a quasi-steady bubble shape treatment.

2.3.4 Transient particle drag

The drag models derived for the motion of a single particle are used in the Euler-Lagrange and Euler-Euler simulation of bubble columns to model the momentum exchange between the gas and liquid phases. In this context, they serve to account for momentum closure and the origin of these models is therefore important in understanding the simulation of bubble columns.

Boussinesq [1885] was the first to derive an analytical expression for the transient hydrodynamic force exerted by a viscous fluid on a solid sphere. He made use of the creeping flow assumption and therefore the model is only valid in the case of extremely small Reynolds numbers (i.e., $Re \ll 1$). The equation consists of three terms i.e., a quasi-steady term, an added mass term and a history term. The quasi-steady term is identical to the steady-state drag derived previously by Stokes [1851]. The added mass force is due to the influence of the acceleration of the surrounding fluid. Finally the history force stems from the temporal delay in boundary layer development as the relative velocity changes with time [Crowe et al., 1998]. Basset [1888] independently derived the same equation three years later.

Maxey and Riley [1983] derived a more general form of the equation of motion which is valid for a rigid sphere in an arbitrary flow field. The solution has more recently been extended by asymptotic expansion methods by Lovalenti and Brady [1993], however, this solution is still only valid at small Reynolds numbers albeit slightly larger, i.e., $Re < 1$. Lawrence and Weinbaum [1988] followed the procedure by Maxey and Riley [1983] and derived an expression for the equation
of motion of an ellipsoid of small eccentricity. This expression included extra
terms to account for the deviation from spherical shape and modifications of
the previous terms that showed that small deviations from spherical shape are
accompanied by significant changes in the analytical equation of motion. Sy et al.
[1970]; Chisnell [1987] derived a transient equation of motion for the case of a fluid
particle. In general these analytical derivations employ advanced mathematical
techniques and yield integro-differential equations.

The practical application of these equations is limited due to the creeping flow
assumption. In an effort to extend the applicability, Odar and Hamilton [1964]
proposed separating the transient creeping flow solution into individual force
contributions (e.g., Eq. 2.20) and multiplying with correction functions correlated
to experimental data. It should be noted that the form of the analytical force
expressions (e.g., Eq. 2.19) is dependent on the corresponding assumptions, with
different assumptions (e.g., non-spherical particle) resulting in disparate force
expressions [Michaelides, 2003]. The physical interpretations associated with the
analytical force terms are therefore no longer valid when their range is extended
through the multiplication with correction functions [Mei and Adrian, 1992]. This
approach has however become popular with engineering calculations in the last
30 years, since the results correlate with experimental data, even though there is
no general agreement on the correction functions themselves [Michaelides, 2003].

\[
m_b \frac{d\mathbf{v}_b}{dt} = 3\pi \mu d (\mathbf{u} - \mathbf{v}_b) + V_b (\nabla p + \nabla \cdot \tau) + \frac{\rho V_b}{2} \left( \frac{D\mathbf{u}}{Dt} - \frac{D\mathbf{v}_b}{Dt} \right) + m_b g \tag{2.19}
\]

\[
m_b \frac{d\mathbf{v}_b}{dt} = \mathbf{F}_D + \mathbf{F}_B + \mathbf{F}_A + \mathbf{F}_H + \mathbf{F}_G \tag{2.20}
\]

The uncertainty in the choice of correction functions transcends into the choice
of closure models for bubble columns simulation since it is possible for closure
models to be applied in regions where they are not applicable. Furthermore,
the solution of the integro-differential equations must be solved by an iterative
Chapter 2. Literature Review

numerical method and is therefore a source of computational expense (in terms of both CPU time and memory) that becomes especially restrictive when considering large numbers of particles in a Lagrangian framework. The choice of terms to include is therefore often based upon the associated computational expense rather than physical correctness. The selection of closure models is generally justified with overall correlations with experimental data, however a more fundamentally based approach would be of interest.

2.4 Simulation of bubble columns revisited

The simulation of bubble columns was briefly discussed in Section 1.4. A more detailed review is presented here. Early treatment of bubble column modelling included a simple plug flow model, superimposed by a diffusional process. Devanathan et al. [1995] noted that due to the transient nature of the flow inside bubble columns this model has no physical base. Other approaches included circulation cell models [Joshi and Sharma, 1979; Zehner, 1982] and gas hold up models [Hill, 1974; Ueyama and Miyachi, 1979] that sought to match macro experimental observations with simple flow models. These simple models lack the capability of the predicting detailed physical descriptions required for the design and optimisation of bubble columns. Furthermore, the recirculating flow structures described by the circulation cell models are not stationary and continuously change location, size and number, due to the transient nature of flow in bubble columns [Lapin and Lübbert, 1994]. In light of these issues, CFD has become a promising tool capable of providing detailed information of the entire transient flow field and thanks to increasing computational capability is becoming popular for the simulation of commercial process engineering applications [Laín et al., 1999].

The first multiphase CFD models used for the simulation of bubble columns originated from the Los Alamos science laboratory [Hirt, 1968; Hirt et al., 1974; Harlow and Amsden, 1975] and were based on finite difference discretisation. One of the key concepts that allows the solution of the Navier-Stokes equations with respect
to velocity and pressure as primitive variables, stems from solving pressure by way of the mass conservation equation, which is known as pressure-velocity coupling. The numerical algorithm for pressure-velocity coupling [Pantankar, 1980] was pioneered at the Imperial College of London and formed the foundation of the first commercial CFD code, PHOENICS. The programming complexity and validation requirements of CFD has led to a demand for more general purpose CFD packages, especially for industrial users. A number of commercial CFD packages have since been developed (e.g., Fluent, CFX, Star-CD). These packages are mostly based on the finite volume method and include state-of-the-art multiphase flow and turbulence models that have been used by various research groups (e.g., Sanyal et al. [1999]; Pfleger and Becker [2001]; Buwa et al. [2006]). Some research groups (e.g., Thakre and Joshi [1999]; Hu [2005]) use in-house code that allow for unrestricted flexibility to introduce novel techniques. Opensource and free-to-use CFD code, most notably OpenFoam [Weller et al., 1998], offer the full flexibility of source code with the advantage of a pre-validated solver for basic cases, however the use of such code requires programming knowledge.

The simulation of gas-liquid flow in bubble columns can be treated with three distinct approaches (i.e., Direct Numerical Simulation, Euler-Lagrange and Euler-Euler), each approximating the flow at different time and length scales (see Figure 1.4). These approaches will be considered in the following sections.

2.4.1 Direct numerical simulation

Direct Numerical Simulation (DNS) refers to the computation of complex unsteady flow where all continuum time and length scales are fully resolved [Tryggvason and Balachandar, 2007]. It follows that DNS can also refer to the simulation of turbulence at very small time and length scales without Reynolds averaging of the Navier-Stokes equations. In the context of bubbly flow, DNS is used to refer to the resolution of gas-liquid flow at the bubble scale where the flow within each phase and interactions are found by solving the Navier-Stokes equations and the bubble shape is part of the solution. This allows the extraction of information that would otherwise be impossible to obtain and has been mainly employed by
the research community to gain insight into multiphase flow phenomena. Due to the extreme computational resource requirements, the DNS simulation of industrial scale gas-liquid flow will remain infeasible for the foreseeable future.

Most of the issues with DNS arise from the drastic change in flow properties occurring at the gas-liquid interface which are sometimes referred to as “jump conditions” [Hua and Lou, 2007]. The numerical representation of these discontinuities are the cause of singularities that require special treatment. Hyman [1984] classified these treatments into moving mesh methods (moving control volumes aligned with the interface), surface tracking methods (following the surface interface using marker points) and volume tracking methods (calculation of the fractional volume of each region separated by the interface as they pass over a reference grid). However, no simple rules exist on which methods are most suited to a particular problem.

2.4.1.1 Moving mesh methods

Moving mesh methods (or body-conformal mesh methods) have been successfully applied for the study of small amplitude waves and weakly deformed bubbles [Ryskin and Leal, 1984; Yang and Prosperetti, 2006; Quan and Schmidt, 2007; Tuković and Jasak, 2012]. The interface is treated as a moving boundary where a sharp interface is maintained exactly by adjusting the mesh to fit the interface or to follow the fluid [Hyman, 1984]. This approach allows for the explicit conservation of volume to be enforced.

The major advantage of this method is the explicit treatment of the interface which allows for a highly accurate representation on fine grids and simple analysis of the results. The disadvantages are the extreme computational expense associated with the re-meshing of the grid when the interface undergoes deformations and the special treatment required to handle the merging of two interfaces. Tuković and Jasak [2012] suggested that the development of highly accurate moving mesh methods can be justified by their potential to provide “numerically exact” solutions that can be used to validate solutions based on fixed mesh methods.
Figure 2.8: The moving mesh DNS method potentially offers the highest accuracy, however, re-meshing results in significant computational expense.

2.4.1.2 Surface tracking methods

Surface tracking methods [Unverdi and Tryggvason, 1992; Tryggvason et al., 2001; van Sint Annaland et al., 2006], specify the interface as an ordered set of marker points located on the interface, or by way of a height function. The main advantage of this approach is that the representation of the surface is independent of the representation of the flow field which allow for high resolution interfaces, enabling the tracking of sub-grid-scale structures. Surface tracking methods have the disadvantage that they do not intrinsically conserve the volume of each fluid, however, volume correction methods have been developed to addressed this issue [Hua and Lou, 2007]. Difficulties from this method stem from the dynamic re-meshing of the Lagrangian interface, the mapping of the Lagrangian data onto the Eulerian mesh [van Sint Annaland et al., 2006] and the merging of interfaces. The computational expense of surface tracking is reduced compared to the moving mesh method.
Chapter 2. Literature Review

2.4.1.3 Volume tracking methods

Volume tracking methods rely on either massless particles (Marker And Cell method (MAC)) or an indicator function (sometimes called colour function) to mark the different fluids or phases. The MAC method is one of the earliest volume tracking methods [Hyman, 1984] and can be prone to artificial numerical diffusion near interfaces. This makes MAC methods harder to generalize for complicated interfaces in multiphase flow and requires many marker particle per computational cell to maintain a well defined interface.

The use of an indicator function, in particular, the use of a fractional volume function (also known as the Volume Of Fluid (VOF) method), has been the subject of many studies (e.g., Krishna and van Baten [1999]; Lörstad and Fuchs [2004]; Dijkstraizen et al. [2005]; Rabha and Buwa [2011]) and is implemented in the major commercial CFD packages. The interface is defined by calculating the fractional volume occupied in each computational cell with the interface occurring in cells with fractional volume (Figure 2.10). The continuum surface force formulation proposed by Brackbill et al. [1992] is a popular approach used to calculate the surface tension force from the distribution of the indicator function. Due to the
nature of the fractional volume distribution, these methods are less capable of producing sharp interfaces compared to the moving mesh and surface tracking methods, however they can straightforwardly account for the merging and interaction of interfaces and are therefore well suited for the studying of bubble breakup and coalescence. In addition, volume conservation can be enforced.

Figure 2.10: The volume fraction distribution function is used to approximate the interface with the volume of fluid volume tracking method.

In a recent study, Krishnan et al. [2010] compared the performance of different numerical discretisation schemes used with the VOF method across the entire bubble flow map (see Figure 2.5). They found large discrepancies between the different schemes. Specifically, the first order upwind scheme with node based gradients was found to significantly outperform those based on higher order discretisation schemes and cell based gradient computations. These findings highlight the uncertainty that exists even with one of the most fundamentally based simulation approaches.


## 2.4.2 Euler-Lagrange

The Euler-Lagrange simulation approach (also known as the trajectory approach and the discrete particle model) can be applied at larger time and length scales and for larger numbers of particles than is currently practical with the DNS methodologies described in Section 2.4.1 (Figure 2.11). The two-phase flow system is approximated as a quasi-homogeneous phase on an Eulerian grid within which each particle (i.e., solid and fluid particles) of the dispersed phase is explicitly tracked by its centre of mass in a Lagrangian framework. The explicit treatment of individual particles allows for the direct consideration of mass transfer, heat transfer, bubble coalescence and a deterministic particle size distribution [Joshi, 2001]. Due to the deterministic location of each particle being stored, Deen et al. [2004] suggested the use of the Euler-Lagrange model for the study of bubble-bubble interaction effects.

![Figure 2.11: Particle tracking of the Euler-Lagrange approach.](image)

Individual bubbles are tracked based on their equation of motion which is governed by the Lagrangian description of Newton’s second law. The force contributions are based on the empirical models for individual particles as discussed in Section 2.3.4. The complexity of the resulting simulation can be classified with respect to the coupling between the phases:

---

37
One-way coupling: The continuous phase influences the motion of the particles, however, the particles have no effect on the continuous phase. This approximation is valid for very small particles in sufficiently dilute systems. A one-way coupled system with an initially stagnant fluid will remain stagnant even with the presence of rising bubbles.

Two-way coupling: Both particle and fluid influence each other i.e., the momentum of the dispersed phase is represented by a source term in the continuous phase momentum balance based on Newton’s third law (i.e., the individual drag forces experienced by the particles act with equal magnitude but in opposite direction on the continuous phase, actio=reactio [Jakobsen, 2008]).

Four-way coupling: Particle-fluid interaction is considered both ways with the addition of particle-particle interaction e.g., particle-particle collisions and coalescence.

The studies by Webb et al. [1992]; Trapp and Mortensen [1993]; Lapin and Lübbert [1994] are some of the first published research utilising the Euler-Lagrange approach for the simulation of bubble columns and is based on a 2D rectangular geometry and a small number of bubbles with differing coupling effects. Delnoij et al. [1997] significantly increased the number of bubbles and included four-way coupling effects for a 2D rectangular bubble column, followed later by a 3D simulation of the same case [Delnoij et al., 1999]. Lain et al. [1999, 2002] accounted for turbulent effects by solving the 2D axisymmetric Reynolds Averaged Navier-Stokes equations for the continuous phase and found the bubble source terms to have a significant effect on the topology of the liquid flow and showed the presence of a bubble size distribution can significantly effect velocity fluctuations. More recently, investigations into 3D models including turbulent effects have been conducted [Buwa et al., 2006; Hu and Celik, 2008; Ali and Pushpavanam, 2011] which show agreement of the time-averaged quantities (e.g., gas hold up) with experimental results, however, uncertainty exists with respect to the choice of bubble source terms, grid resolution and turbulence effects. The major issue with the Euler-Lagrange approach follows from the proportional increase in computational expense with number of particles (due to a separate equation of motion to be solved iteratively for each particle) which becomes prohibitive for
the simulation of high volume fraction bubble columns [Ali and Pushpavanam, 2011].

2.4.3 Euler-Euler

The Euler-Euler approach (or two-fluid approach) treats both phases as interpenetrating continua on an Eulerian grid, resulting in a separate momentum balance equation for each phase. The phases are volume averaged (also referred to as ensemble averaged) over space such that a phase fraction is introduced into the equation set. This fraction is defined as the probability that a certain phase is present at a given point in space and time (Figure 2.12). The presence of the dispersed phase is subsequently deduced from the spatial phase fraction distribution. The momentum transferred between the phases (or the momentum closure) is modelled based on the particle drag as discussed in Section 2.3.4. The choice of which force contributions to include is (as in the case of the Euler-Lagrange approach) often based on computational expense and the subject of debate in the field of multiphase flow [Sokolichin et al., 2004].

![Figure 2.12: Volume averaging of the Euler-Euler approach.](image)

The early Euler-Euler bubble column simulations were performed at steady-state
Chapter 2. Literature Review

[Torvik and Svendsen, 1990; Grienberger and Hofmann, 1992; Jakobsen et al., 1993; Hillmer et al., 1994]. Sokolichin and Eigenberger [1994] were amongst the first to present simulation results for an unsteady 2D rectangular bubble column and noted that the transient simulation of bubble columns exhibits substantially different behaviour to the steady state simulations and appears more in line with experimental observations. Subsequent investigations (e.g., Sokolichin and Eigenberger [1999]; Borchers et al. [1999]; Bech [2005]) focussed on a similar 2D unsteady rectangular bubble column which has been named the “Becker test case” after the detailed experimental results from the study of Becker et al. [1994]. Pfieger and Becker [2001] reported the simulation of a 3D cylindrical bubble column, where it was concluded that fine grids are necessary to obtain accurate results. These high resolution grids come at the cost of enormous computational expense and a compromise between grid density and computational effort is therefore required.

Sokolichin et al. [1997]; Ali and Pushpavanam [2011] compared the Euler-Euler simulations to that of Euler-Lagrange simulations on rectangular bubble columns and reported that the Euler-Euler approach is the most suited for the simulation of high gas fractions operating range. Rafique and Dudukovic [2006] investigated the influence of different closure models on the hydrodynamics of bubble column flows. They found most of the drag models investigated yielded reasonable engineering estimates of the liquid recirculation velocity profile, however, the gas-holdup was found to be sensitive to the choice of drag model with no clear “best choice” due to lack of accurate experimental gas-holdup profiles.

It is generally accepted that the Euler-Euler approach is the most suitable approach to simulate industrial scale bubble column reactors due to the applicability to high gas fraction flows and the use of relatively coarse grids [Sundaresan, 2000]. The implementation of a bubble size distribution is however not straightforward as with the Euler-Lagrange case. Lo [1996] was the first to introduce a bubble size distribution into the Euler-Euler approach by way of population balance modelling through his MUltiple-SIze-Group model (MUSIG). Each size

---

1 An introduction to population balance modelling is presented by Ramkrishna [2000].
2 The term MUSIG is however, not popularly used and researchers more often refer to the
group requires an additional set of momentum equations to be solved which sub-
stantially increases computational requirements. The size distribution of the dis-
persed phase is often very important since all inter-phase transport phenomena
are governed by the mean area concentration [Sundaresan, 2000] and therefore
the PBM-EE approach has become the subject of intensive research (e.g., Chen
et al. [2004]; Yeoh and Tu [2004]; Wang et al. [2005]; Bhole et al. [2008]; Cheung
et al. [2008]). The interest in the PBM-EE approach has also resulted in increased
research into the breakup and coalescence of bubbles since these models can be
incorporated within a population balance framework [Mitre et al., 2010].

2.5 The finite volume method

The discretisation of the transport equations is central to the numerical simula-
tion of fluid flow, whereby partial differential equations are transformed into cor-
responding algebraic equations. At first, the solution domain is discretised into a
finite number of non-overlapping elements (i.e., mesh generation). The equations
can subsequently be discretised over the domain, where the most important ap-
proaches are the finite difference, finite volume and finite element methodologies
[Ferziger and Perić, 1999]. The finite volume method is based upon the volume
integral formulation of the governing equations and is therefore inherently con-
servative. Furthermore, this method is well suited to unstructured grids and is
less memory intensive than the finite element method, which contributes to its
popular use in commercial CFD codes. The discretisation of the general trans-
port equation, according to the finite volume methodology, is examined in the
following subsections.

2.5.1 Discretisation

The transformation of mathematical operators into arithmetic operators that
can be processed by computers, is examined by way of the finite volume method.
Chapter 2. Literature Review

For this purpose, the standard transport equation for either a scalar or a vector quantity, \( \phi \), is examined in Eq. 2.21.

\[
\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi \tag{2.21}
\]

The finite volume formulation is attained by integrating Eq. 2.21 over a given control volume, \( dV \), and timestep, \( dt \) (Eq. 2.22). The discretisation of the individual terms arising from the volume and time integration is considered in the following sections.

\[
\int_t^{t+\Delta t} \left[ \int_V \frac{\partial \rho \phi}{\partial t} dV + \int_V \nabla \cdot (\rho \mathbf{u} \phi) dV \right] dt = \int_t^{t+\Delta t} \left[ \int_V \nabla \cdot (\Gamma \nabla \phi) dV + \int_V S_\phi dV \right] dt \tag{2.22}
\]

2.5.1.1 Time derivative

Implicit discretisation of time has the advantage of stability over much larger time steps compared to explicit methods [Anderson, 1995]. The Euler implicit differencing scheme, Eq. 2.23 (the superscript \( p \) here refers to values from the previous time step), is first order accurate and often employed in CFD codes. Higher order time differencing schemes may be employed, however, requires the overhead of storing data for additional time steps. The Euler implicit temporal discretisation will be assumed for the spatial terms as well, thereby implying \( \phi \) to refer to the latest time values.

\[
\int_V \frac{\partial \rho \phi}{\partial t} dV \approx \frac{\rho \phi - \rho^p \phi^p}{\Delta t} V \tag{2.23}
\]
Chapter 2. Literature Review

2.5.1.2 Convection

Discretisation of the convection term can be achieved through transformation of the volume integral into a surface integral by invoking Gauss’ theorem (also called the divergence theorem). This theorem states that the outward flux of a vector field through a closed surface is equal to the volume integral of the divergence of the region inside the surface, which in essence describes the conservation of a tensorial quantity. Subsequently, the volumetric quantities can be approximated as the sum of the outward fluxes at control volume faces (Eq. 2.24).

\[
\int_V \nabla \cdot (\rho u \phi) dV = \oint_{S_f} \mathbf{S}_f \cdot (\rho \mathbf{u} \phi) \approx \sum_{f}^{n_{faces}} \mathbf{S}_f \cdot (\rho \mathbf{u} \phi) \quad (2.24)
\]

2.5.1.3 Diffusion

The discretisation of the diffusion term, similar to the convection term, can be treated by applying Gauss’ theorem (Eq. 2.25).

\[
\int_V \nabla \cdot (\Gamma \phi \nabla \phi) dV = \oint_{S_f} \mathbf{S}_f \cdot (\Gamma \nabla \phi) \approx \sum_{f}^{n_{faces}} \Gamma_{\phi,f} (\mathbf{S}_f \cdot \nabla \phi) \quad (2.25)
\]

To compute the face gradient term, \(\nabla \phi\), the difference of \(\phi\) between the present cell \((P)\) and a neighbouring cell \((N)\) is divided by the norm of the vector between the cell centres \(d\). This formulation can be used directly for orthogonal grids, however, for non-orthogonal grids a explicit correction term is introduced which has been subject to intensive research\(^1\).

\[
\nabla \phi = \frac{\phi_N - \phi_P}{|d|} \quad (2.26)
\]

\(^1\)The reader is referred to Ferziger and Perić [1999] or Jasak [1996] for the treatment of the non-orthogonal correction term
2.5.1.4 Source

The discretised equations will be expressed as a linear system of equations and to aid in achieving a diagonally dominant coefficient matrix, which improves the conditioning of the system of equations, the source term is linearised into implicit and explicit contributions (Eq. 2.27).

\[ S_\phi = \phi S_{\phi,I} + S_{\phi,E} \]  

(2.27)

The resulting terms are integrated over a control volume, yielding Eq. 2.28.

\[ \int_V S_\phi dV = S_{\phi,I} V \phi + S_{\phi,E} V \]  

(2.28)

2.5.1.5 Discretised transport equation

Combining the discretised terms obtained from the previous sections i.e., Eq. 2.23 - 2.28 into Eq. 2.22, the semi-discretised form of the transport equation can be expressed (Eq. 2.29). Other discretisation methodologies are examined by Hirsch [2007].

\[ \int_t^{t+\Delta t} \left[ \frac{\rho \phi - \phi^p}{\Delta t} V + \sum_{f} S_f (\rho u \phi) \right] dt = \int_t^{t+\Delta t} \left[ \sum_{f} \Gamma_{\phi,f} (S_{\phi,f} \cdot \nabla f \phi) + S_{\phi,I} V \phi + S_{\phi,E} V \right] dt \]  

(2.29)

The final discretised transport equation, following integration of time, is given in Eq. 2.30.

\[ \rho \frac{\phi - \phi^p}{\Delta t} V + \sum_{f} S_f (\rho u \phi) = \sum_{f} \Gamma_{\phi,f} (S_{\phi,f} \cdot \nabla f \phi) + S_{\phi,I} V \phi + S_{\phi,E} V \]  

(2.30)
Chapter 2. Literature Review

2.5.1.6 Algebraic equation system

The discretisation procedures from the preceding subsections transform the partial differential transport equations into a set of linear algebraic equations for each control volume within the discretised domain. The resulting equation for an individual cell can be written in terms of a coefficient for the present cell \( a_P \), neighbouring cells \( a_N \) and a source term \( R_P \) as given in Eq. 2.31.

\[
a_P \phi_P + \sum_N a_N \phi_N = R_P
\]  

(2.31)

The algebraic equations for all the cells in the domain can be expressed in matrix form as depicted in Eq. 2.32, where \([A]\) is the matrix of coefficients and \([R_m]\) represents the source vector.

\[
[A][\phi] = [R_m]
\]

(2.32)

Here implicit terms contribute to the matrix coefficients while explicit terms only contribute to the source vector. The system of equations is subsequently solved with an appropriate numerical technique to yield a solution for \( \phi \). This can be achieved in two ways i.e., direct or iterative methods [Ferziger and Perić, 1999]. In general iterative methods are better suited for CFD application, since they can take advantage of sparse matrices, thereby reducing memory requirements, and are less computationally expensive to evaluate compared to direct methods that yield exact solutions at high computational expense for large grids.

2.5.2 Solution of the Navier-Stokes equation

The solution of the momentum transport equation i.e., \( \phi = \rho u \) in Eq. 2.21, present two issues that require special treatment. Firstly, the convection of momentum is a non-linear term which arises from the multiplication of velocity with the velocity gradient. This problem is treated by lagging one of the velocities from the previous time step, which requires the time step to be sufficiently small.
Chapter 2. Literature Review

[Kärrholm, 2008]. The second issue is that there is no explicit equation for pressure. This problem is overcome by employing a pressure-velocity coupling scheme which derives an equation for pressure. The scheme presented here is based upon the pressure-velocity coupling used in the transient incompressible flow simulation of OpenFoam [Weller et al., 1998].

Following from the cell-wise algebraic equation (Eq. 2.31), define the operator \( H \) as the sum of the source term excluding pressure \( (R^p) \), and the neighbouring cells contribution (Eq. 2.33). The algebraic equation can subsequently be rewritten with respect to the \( H \) operator, Eq. 2.34 and 2.35.

\[
H = R^p - \sum a_N u_N \quad (2.33)
\]
\[
a_P u_P = H - \nabla P \quad (2.34)
\]
\[
u_P = \frac{H - \nabla P}{a_P} \quad (2.35)
\]

Applying the divergence operator to both sides of Eq. 2.35, and recognizing that \( \nabla \cdot u_P = 0 \) since the flow is assumed incompressible, yields the Poison Pressure Equation (PPE), Eq. 2.36.

\[
\nabla \cdot \left[ \frac{\nabla P}{a_P} \right] = \nabla \cdot \left[ \frac{H}{a_P} \right] \quad (2.36)
\]

The term \( \frac{H}{a_P} \) can be viewed as velocity without the effect of pressure [Ferziger and Perić, 1999] and the values are interpolated from the cell centres to the cell faces. This interpolation is done in the spirit of Rhie and Chow [1983] to allow for a collocated grid arrangement that does not result in the “checker-board” pressure solution [Versteeg and Malalasekera, 2007]. The application of a Rhie-Chow type correction is essential for flow simulations on a collocated grid and is therefore used in most modern CFD codes.
Chapter 2. Literature Review

2.6 Design and Analysis of Computer Experiments

The Design and Analysis of Computer Experiments (DACE) methodology was introduced by Sacks et al. [1989] as a way of approximating complex computer models with more efficient predictors by modelling the deterministic output as the realization of a stochastic process $Y(x)$ that includes a regression model of $n$ chosen functions $f_i$ with regression coefficients $\beta_i$ and a random process $Z(x)$ (see Eq. 2.37). The method focusses on modelling the error as opposed to the functional form of the regression model.

From a modelling perspective, the key difference between physical experimental data and that produced by a computer experiment is that the latter is effectively free from random error (except for truncation errors, or if this is simulated e.g., random sampling), and the error can be attributed due to lack of fit [Jones et al., 1998]. It is this distinction that allows computer experiments to be approximated more accurately in a way that predicts non-linear responses and other complex behaviour, which in many cases becomes a futile task with physical data due to random noise.

Since the error in the model is due to the lack of fit of the regression function, spatial dependence of the error may be assumed, which implies that when two points are close to each other, their errors should be close as well. The form and the weight of this dependence will depend on the behaviour of the data being fitted. Therefore, DACE is aimed at estimating how a function typically behaves in contrast to regression, which estimates the weighting on an assumed functional form, thereby estimating what the function is [Jones et al., 1998]. The response can be written in the form of Eq. 2.37 with the expected value (where $E[\cdot]$ refers to the expected value [Ross, 2007]) of the random process as zero and the expected variance, $\sigma^2\mathcal{R}$, where $\mathcal{R}$ represents the covariance matrix (Eq. 2.38).
Chapter 2. Literature Review

\[ Y(x) = \sum_{i=1}^{n} f_i(x) \beta_i + Z(x) \]  
\[ E[Z(x)] = 0, \quad E[Z(x)Z(x)^T] = \sigma^2 R \]  

In the case of simple least squares, \( \mathbf{R} \) will correspond to the identity matrix. This model is a generalized least squares implementation, where the off-diagonal entries of \( \mathbf{R} \) is modelled by a correlation function. For a given set of sample points, \( S = [s_1, \ldots, s_{n_{\text{samp}}} \] , a method known as Kriging [Krige, 1951] has been established which describes the prediction at some point \( x \) as the linear combination of sampling responses \( Y_S = [Y(s_1), \ldots, Y(s_{n_{\text{samp}}})] \), Eq. 2.39.

\[ \hat{y}(x) = c^T(x)Y_S. \]  

Minimizing the mean squared error (MSE) of the predictor subject to the unbiasedness constraint and solving for \( c(x) \) results in the Best Linear Unbiased Predictor (Eq. 2.40). Here \( \hat{\beta} = \mathbf{F}^T \mathbf{R}^{-1}Y_S(\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \) is the generalized least squares estimate of \( \beta \) [Santner et al., 2003]. Here \( \mathbf{F} \) corresponds to the regression function evaluated at \( S \), and \( r \) the vector of correlations between the sample points, \( S \), and the prediction point \( x \). Please refer to Sacks et al. [1989] for a detailed derivation of the model. The Best Linear Unbiased Predictor will in this study be referred to as the the DACE model.

\[ \hat{y}(x) = f^T(x)\hat{\beta} + r^T(x)\mathbf{R}^{-1}(Y_S - F\hat{\beta}) \]  

It follows that the DACE model predicts the response as the linear combination of the sampling responses (Eq. 2.39), where the influence of each sample response is determined by a distance dependant correlation function. The DACE model can therefore be seen as an optimal interpolator, whose parameters are represented by those of the correlation function.
2.6.1 Correlation function

The form of the correlation is extremely important as it has to be able to capture the behaviour of the data. The requirement is generally that the correlation approaches zero as the distance between two points approaches infinity, and approaches one as the distance approaches zero. This behaviour is given by the flexible functional form of the powered exponential correlation for \( n_d \) dimensional data, Eq. (2.41), which is also referred to as the Kriging basis function [Jones, 2001].

\[
\mathcal{R}_{ij} = \exp\left(-\sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}|^{p_k}\right) \tag{2.41}
\]

The \( \Theta \) parameters correspond to the activity while \( p \) represents the smoothness of the correlation. Different activities can be used for each dimension which is known as anisotropic behaviour, and allows the form of the correlation function to vary depending upon the approaching direction. For \( p = 2 \) the correlation function will correspond to the Gaussian correlation, which is smooth, while for \( p = 1 \) the correlation will be linear.

Another popular correlation is known as the Matérn covariance function, given in Eq. 2.42. Here \( K_p \) is a modified Bessel function of the second kind of order \( p \), and \( \Theta \) and \( p \) carry the same significance as in equation (2.41). It is also known as the Whittle-Matérn function since it was introduced by Matérn [1960] but was derived earlier by Whittle [1954]. The correlation can produce ill-conditioned covariance matrices for certain \( p \) parameters and therefore it might be preferred to optimise a discrete set of \( p \) [Diggle, 2007].

\[
\mathcal{R}_{ij} = \frac{1}{2^{p-1}\Gamma(p)} \left(\sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}|\right)^p K_p\left(\sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}|\right) \tag{2.42}
\]
Chapter 2. Literature Review

2.7 Critical summary

From the literature presented, specific key aspects can be emphasized. It is well known that fluid flow can be described by the Navier-Stokes equations, which follows from assuming the domain as a continuum in time and space and applying conservation principles. To solve the subsequent equations, either simplifying assumptions need to be made to obtain analytical solutions or the equations need to be discretised in space and time and solved numerically. For a numerical solution, the finite volume method is particularly attractive since it is inherently conservative and well suited to unstructured grids.

The Design And Analysis of Computer Experiments (DACE) methodology models the covariance between a selection of sample points and has been shown to accurately approximate complex surfaces with little knowledge of the underlying process. Subsequently this approach has the potential to construct surrogate models of non-linear surfaces produced by CFD.

The key factors influencing the rise characteristics of a bubble i.e., fluid properties, size and velocity can be summarized by dimensionless numbers that can ultimately be used to determine the state of a bubble. The boundary condition at the surface of a bubble corresponds to a zero-shear-stress condition which differs from a rigid object and influences the drag force and resulting flow field.

The modelling of gas-liquid flow occurring in bubble columns has been treated with one of three distinct approaches i.e., Euler-Euler, Euler-Lagrange and Direct Numerical Simulation (DNS), where each simulates multiphase flow at different time and length scales, while computational expense increases in accordance with the level of flow information being generated. With current computational resources it is infeasible to simulate more than a few bubbles at the bubble scale (i.e., following the DNS approach) due to computational expense. A significant amount of research has been conducted into these approaches leading to improvements in prediction accuracy and the size of the problems being studied. However, computational expense remains a major factor inhibiting the simulation of bubble scale flow at larger geometries.
Chapter 3

Thesis Objectives

The simulation of bubble columns is of interest to both commercial entities and academic researchers due to their common usage as process reactors and the challenge posed by their complex hydrodynamics. Methodologies for simulating bubble-liquid interaction at different length scales have been employed (as reviewed in Section 2.4) that rely on the numerical solution of the Navier-Stokes equations. However, computational expense remains a formidable barrier that restricts the application of these models, particularly the simulation of bubble scale flow information at reactor scale geometries. Furthermore, although the computational performance of computers has increased exponentially over the past six decades, the demands of frontier flow simulations have never been satisfied and the historical computational performance growth is not guaranteed to continue indefinitely.

The primary contribution of this study is the development of a novel two-phase simulation approach that can be applied to bubbly flows. The aim of this approach is the prediction of small scale flow detail at significantly reduced computational demand. The essential concept of this technique is stated below.

For the development of a computationally efficient, fundamentally based bubble flow simulator, it is proposed to substitute the high gradient regions around individual bubbles, within an Euler-Lagrange framework, with a surrogate model that can be rapidly evaluated.
Chapter 3. Thesis Objectives

The development of the surrogate model constitutes a major contribution from this study since the lack of a suitable model could be regarded as the primary impediment towards the application of the proposed approach. The surrogate model will be referred to as the Bubble Cell Model (BCM) since the immediate flow fields around individual bubbles are treated explicitly as the “cells” which form the fundamental building blocks of the simulation (Figure 3.1). For the purpose of this study, i.e., a proof of concept, bubbles will be assumed spherical for which the parameters are the Reynolds number, spatial position ($x$) and model coefficients ($\gamma$).

![Figure 3.1: The Bubble Cell Model (BCM) concept, the subject of this study.](image)

The construction of the surrogate model is treated with a two-stage process whereby the first stage entails approximating the spatial velocity field, while the second stage involves the Reynolds number dependence of the model. The two key requirements of the surrogate model are accuracy and rapid evaluation. Statistical modelling is therefore justified and the DACE model (examined in Section 2.6) is applied to approximating the spatial velocity fields at discrete Reynolds numbers (Chapter 4). The use of simplified analytical solutions are subsequently investigated to improve stage one model accuracy and reduce the
number of model parameters in Chapter 5. The Reynolds dependence is examined during the second stage construction in Chapter 6. Finally the coupling of the BCM with flow field outside of its spatial range is considered in Chapter 7 and evaluated for two test cases.

To the author’s knowledge, this study is a first of its kind and represents a proof of concept for the proposed simulation approach, which entails the investigation of various model fitting strategies and numerical method aspects. It is therefore considered sensible to focus on the homogeneous flow regime for simple cases while recognising potential for extension of the operating ranges.

Main contributions

The main contribution points of this study is summarised below:

- The application of the DACE methodology for fitting non-linear flow structures produced using CFD. This entails the proposal of novel correlation functions and sampling design strategies.

- The combination of analytically-inspired and purely statistical formulations to model the flow structures around a spherical bubble.

- The development and application of a two-stage fitting strategy to yield a model (the BCM) that describes the micro-scale flow field around a spherical bubble as a function of Reynolds number.

- The development of a CFD simulation framework that imposes the flow fields predicted by the BCM in the regions surrounding individual bubbles.

- Significantly reducing the computation time for the simulation of bubble induced flow within the operating range of the BCM.
Chapter 3. *Thesis Objectives*
Part II

Model Development
Chapter 4

Preliminary bubble flow model investigation

The stage one construction of a bubble flow model capable of rapidly and accurately predicting the velocity flow field around a bubble at discrete Reynolds numbers, forms a crucial part of the proposed bubble column simulation approach. In the present chapter, the Design and Analysis of Computer Experiments (DACE) methodology (surveyed in Section 2.6) is applied to approximating the velocity flow fields at 5 discrete Reynolds numbers to establish the feasibility of this modelling approach to the given data. The focus falls on identifying the best combinations of sampling designs and correlation functions and therefore only the primary velocity field (i.e. the $y$ velocity field, based on the solution of the 2 dimensional Navier-Stokes equations) will be considered in this chapter to save computational time in fitting the surfaces.

The stage one BCM construction process is described in Section 4.1 followed by an examination of the simulation that is to be approximated in Section 4.2. The DACE modelling approach together with corresponding correlation functions and parameter estimation strategies is considered in Section 4.3. Different sampling designs are introduced in Section 4.4, followed by the presentation and analysis of results in Section 4.5. Finally, conclusions regarding this preliminary investigation are drawn in Section 4.6.
4.1 Bubble Cell Model: Stage one introduction

The flow structure around a bubble can be generated by solving the Navier-Stokes equations for the flow over a fixed sphere. This approach is similar in concept to the relative velocity principle used in analysing wind tunnel experiments that was remarkably first suggested by Leonardo, who stated: “As it is to move the object against the motionless air so it is to move the air against the motionless object” and “The same force as is made by the thing against the air, is made by air against the thing” in the codex Atlanticus [Anderson, 2010]. In the context of the construction of the BCM, this can be viewed as the computer experiment which is conducted for different relative velocities ($u_{rel}$). These relative velocities together with the fluid properties of the continuum can be parametrised by the Reynolds number ($Re$) to develop a model that can be applied for any gas-liquid system within the operating range. It should be noted that there is potential to account for different shaped bubbles, as discussed in Section 2.3.1, through the use of the dimensionless Eötvös, Weber and Morton numbers, however, for the present study the model will be restricted to the spherical case.

The first stage development of the BCM entails approximating the flow fields from the BCM experiment with respect to spatial position at different Reynolds numbers. The intended application of the BCM is the simulation of gas-liquid flows occurring in bubble columns by updating the flow field around individual bubbles at each reactor time step for a given Reynolds number. The concept of approximating the flow field around individual bubbles based on the Navier-Stokes simulation of the flow over a fixed sphere is illustrated in Figure 4.1. It follows that the BCM is the fundamental building block upon which the bubble column simulation is built and therefore its accuracy is essential to the prediction accuracy of the resulting BCM-based simulation. Furthermore, given that the parameters of the spatial flow model is set to under-go cross correlation with respect to $Re$ (that will inherently further error), exemplifies the need for accurate first stage models.

The development of the first stage BCM essentially translates into a study of fitting complex surfaces. The Design and Analysis of Computer Experiments
Chapter 4. *Preliminary bubble flow model investigation*

Figure 4.1: The macro model uses the information provided by the BCM to update the flow field around each bubble in the column. The BCM is based on the Navier-Stokes solution of the analogous situation of flow over a sphere which constitutes the BCM experiment.
(DACE) is a statistical approach that can be used to develop an useful understanding of how model responses are related to model inputs [Santner et al., 2003]. The predictor resulting from the DACE approach, is dependent on the model inputs and responses at specified sample points and can therefore be described as an optimal interpolator. The DACE approach has been successfully applied to optimise expensive black-box functions [Jones et al., 1998] and in shape optimisation using CFD simulations in the field of aeronautics [Marsden et al., 2004; Jouhad et al., 2007]. Some key advantages to using the DACE model are its flexibility to any data type, its ability to describe non-linearity and the potential to work with high dimensional data. In the context of the BCM, the DACE approach is effectively a regression of high resolution data. Before DACE can be applied the generation of the velocity flow field data will be considered in the following section.

### 4.2 Flow field data generation

The Navier-Stokes equations describe the motion of fluids [Batchelor, 1967] and their solution constitute the data to be approximated. The equations are derived by assuming that the fluid is a continuum and applying the principles of conservation of mass and momentum. To complete the equations, the mathematical expression describing the fluid viscosity needs to be assumed. Assuming an incompressible Newtonian fluid at steady state, the equations can be expressed in Cartesian coordinates in dimensionless vector form (the * superscripts denote the dimensionless quantities) as shown in Eq. 4.1 below.

\[
\mathbf{\nabla}^* \mathbf{u}^* = 0 \quad (2.3)
\]

\[
(u^* \cdot \mathbf{\nabla}^*) u^* = -\mathbf{\nabla}^* P^* + \frac{1}{Re} \mathbf{\nabla}^2 \mathbf{u}^* \quad (4.1)
\]

From the literature review presented in Section 2.3.2 it follows that the boundary
condition treatment for the gas-liquid interface of a bubble corresponds to a zero-shear-stress condition for a contaminant free system. This is in contrast to the no-slip treatment of a rigid particle or a fully contaminated bubbly flow system [Magnaudet and Eames, 2000]. Since the BCM is currently being developed for a clean system, the boundary condition on the wall of the fixed sphere will be treated as a zero-shear-stress condition. The Reynolds number operating range is based on the experimental observations for a clean air water system, where the bubble remain spherical around $Re \leq 270$ [Clift et al., 1978]. This range is therefore accepted for the construction of the BCM.

The Navier-Stokes equations are numerically solved utilizing the Finite-Volume method with the SIMPLE pressure-velocity coupling scheme and 2nd order UPWIND spatial discretisation using the FLUENT 12 CFD code. The mesh is set up according to the geometry displayed in Figure 4.2. To allow for accurate flow structures to develop, the resolution of the mesh has to be high enough. This was determined by computing the force on the bubble on consecutively finer grids until no change in the prediction was found. Triangular elements were used since they provide less skewed elements for the given geometry. The velocity and pressure data is therefore available on the grid, which results in 164,983 data points in the sampling region (Figure 4.1).

In order to establish the validity of the simulation results for the flow field approximation of a physical bubble, the drag coefficient resulting from the velocity flow field solutions have been compared with experimental results [Haberman and Morton, 1953] and established drag correlations for a contaminant free system [Moore, 1963; Hamielec et al., 1963] at various Reynolds numbers within the operating range. The simulated drag coefficients are shown to correspond well to the published data in Figure 4.3, although slightly higher at the low Reynolds numbers.
Chapter 4. Preliminary bubble flow model investigation

Figure 4.2: Experimental geometry and mesh, the geometry is set up according to the diameter (D) of the bubble and ratio’s chosen to allow flow dynamics to sufficiently develop across the domain.

Figure 4.3: Comparison of the simulated drag coefficient with experimental results [Haberman and Morton, 1953] and correlation models [Moore, 1963; Hamielec et al., 1963]
4.3 Design and Analysis of Computer Experiments

The Design and Analysis of Computer Experiments approach is discussed in the literature review in Section 2.6. This methodology focuses on modelling the covariance between a set of sample points. This is achieved through the modification of the covariance matrix ($\mathcal{R}$), whereby the off diagonal entries are modelled with appropriate correlation functions. Spatial dependence is thereby assumed and each prediction point represents a weighted linear combination of all the sample points. The weighting is dependent on the correlation function and its parameters, which is discussed in Section 4.3.1 followed by the numerical procedure for constructing the DACE model in Section 4.3.2.

4.3.1 Correlation function

The basic requirements of a correlation function for the modelling of covariance are that the correlation tends to one as the distance between two points approaches zero and that the correlation approaches zero as the distance tends to infinity. The most basic form that exhibits this behaviour is the powered exponential function presented in Eq. 2.41 and repeated below. This correlation function will be referred to as the “EXP” correlation in this chapter. Note, when the number of dimensions is in the same order as the number of sample points, the covariance matrix can be numerically unstable unless it is “regularized” [Bickel and Levina, 2008]. A common method to deal with such problems is “banding” whereby entries of the matrix decay as they move away from the diagonal [Cai and Yuan, 2012]. However, since the number of dimensions ($n_d = 2$) is significantly smaller than the number of samples, this is not considered a problem.

$$
\mathcal{R}_{ij} = \exp\left(-\sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}|^{p_k}\right)
$$

The Matérn correlation function is commonly applied to the model spatial covari-
Chapter 4. Preliminary bubble flow model investigation

ance [Minasny and McBratney, 2005; Diggle, 2007]. It is presented in Eq. 2.42 and repeated below. In this chapter this correlation function will be referred to as “MATERN”. When dealing with this correlation function, the initial conditions of the correlation parameters are adjusted when ill-conditioned covariance matrices are produced to avoid very bad approximations.

\[ R_{ij} = \frac{1}{2^{p-1} \Gamma(p)} \left( \sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}| \right)^p K_p \left( \sum_{k=1}^{n_d} \Theta_k |x_{ik} - x_{jk}| \right) \]  

(2.42)

A modification to the powered exponential correlation (Eq. 4.2) is introduced in this study, that allows the correlation to be dependent on the distance to some point of interest, \( x_c \). This point could potentially represent the point of maximum gradient (optimum) or mark an important feature in the data. This correlation function will be referred to as “EXP-C”.

\[ R_{ij} = \exp\left(- \sum_{k=1}^{n_d} \theta^*_k |x_{ik} - x_{jk}|^{p_k} \right) \]  

(4.2)

with \( \theta^*_k = \theta_k + \theta_k \lambda m(w) \) and \( m(w) \) is the desirability function of the form:

\[ m(w) = \frac{\exp(s) - \exp(s|w|)}{\exp(s) - 1}. \]  

(4.3)

Here \( s \) is the importance or activity of the critical point \( x_c \), while \( w \) can be defined for each dimension as

\[ w_1 = \sum_{k=1}^{n_d} \frac{(x_{ik} - x_{ck})^2}{(x_{max,k} - x_{min,k})^2} \]  

(4.4)

\[ w_2 = \sum_{k=1}^{n_d} \frac{(x_{jk} - x_{ck})^2}{(x_{max,k} - x_{min,k})^2} \]  

(4.5)

The desirability can now be specified as a function of the weighted contribution of \( w_1 \) and \( w_2 \):

\[ m(w) = m(\lambda w_1 + (1 - \lambda)w_2) \]  

(4.6)
Chapter 4. *Preliminary bubble flow model investigation*

For this investigation, the point of interest was chosen as the centre of the bubble, the weighting as $\lambda = 0.5$ and the activity, $s$, set as an optimisation variable. Desirability functions of the form of equation (4.3) is commonly applied to dual response surface optimisation problems [Coetzer et al., 2008].

### 4.3.2 Parameter estimation of correlation functions

To complete the DACE model, the parameters of the correlation function need to be quantified. A popular technique is to assume that the underlying distribution of $Z(\cdot)$ is Gaussian which allows the $\Theta$’s to be estimated such that they maximize the corresponding log likelihood function in terms of the sampled data [Koehler and Owen, 1996]. This ensures that the data being predicted is most likely to have come from the same model as the data from the sample points when the underlying error distribution is Gaussian. This method is known as the Maximum Likelihood Estimation (MLE) of the parameters.

Since high resolution data is being generated from the solution of the Navier-Stokes equation on a fine grid (Section 4.2), there are data points available that could be used for a more accurate estimate of $\Theta$. Furthermore, this allows for the estimation of other correlation parameters such as the smoothness parameter, $p$, and the desirability parameter $s$, as well, which are usually chosen as discrete values. Utilising the high resolution data thereby provides potential for exploring novel correlation functions with the only constraint being the effectiveness of the optimization routine in the light of potential non-linear multi-parameter correlation functions. This investigation therefore, also serves as an test case for the application of the DACE model to summarising high resolution data.

The procedure for constructing the DACE model and estimating its parameters is given:

1. Obtain the velocity field, $Y$, for a given Reynolds number using the CFD experiment discussed in Section 4.2

2. Determine the sampling points and corresponding sample responses $Y_S$ (discussed in Section 4.4)
3. Construct the covariance matrix, $\mathcal{R}$, using a correlation function as discussed in Section 2.6.1 with parameters $\Theta$ and $p$ (for EXP-C include estimation of $s$)

4. Compute the Cholesky decomposition of $\mathcal{R}$ such that $CC^T = \mathcal{R}$

5. Compute the generalized least squares solution for $\hat{\beta}$ using $C$

6. Evaluate the DACE model, $\hat{y}$, at all the grid points of the CFD solution using equation 2.40 with $\mathcal{R}^{-1} = C^{-T}C^{-1}$

7. Compute the mean squared error for the fit i.e. $MSE = mean((Y - \hat{y})^2)$

An optimisation problem is solved for the estimation of parameters $\Theta$ and $p$ (for EXP-C include $s$), where steps 3 to 7 are repeated until the convergence criteria has been met.

### 4.4 Sampling Design

The sampling design, together with the error correlation function, have to represent the entire domain of the non-linear model. Furthermore, a different design may result in an entirely different covariance matrix on the same data set and therefore the best error correlation function will also be dependent on where the points are sampled. It is theoretically possible to regress for the positions of all the points together with the correlation parameters according to the MSE of the predicted response, but this would result in a very high dimensional optimisation exercise which is extremely computationally expensive and unreliable. Therefore, different criteria for generating designs are evaluated to establish what defines a good sampling design for the current problem.

Since the numerically generated data is deterministic, Fisher’s [Fisher, 1935] design of experiments methodology of randomization, replication and blocking become irrelevant. Instead, all the attention can be focused on the location of the sample points. Sampling designs developed specifically for computer experiments...
Chapter 4. *Preliminary bubble flow model investigation*

Table 4.1: Sampling Designs

<table>
<thead>
<tr>
<th>Design</th>
<th>Description</th>
<th>Data Dependent</th>
<th>$n_{samp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RND</td>
<td>Randomly selected points</td>
<td>No</td>
<td>30, 60, 90</td>
</tr>
<tr>
<td>LHD</td>
<td>Latin Hypercube Design (with maximin criteria)</td>
<td>No</td>
<td>30, 60, 90</td>
</tr>
<tr>
<td>UDC</td>
<td>Uniform design in Cartesian coordinates</td>
<td>No</td>
<td>24, 56, 84</td>
</tr>
<tr>
<td>UDP</td>
<td>Uniform design in polar coordinates</td>
<td>No</td>
<td>25, 64, 81</td>
</tr>
<tr>
<td>UTM</td>
<td>Uniform triangulated mesh</td>
<td>No</td>
<td>30, 60, 90</td>
</tr>
<tr>
<td>CPD</td>
<td>Critical Point Design</td>
<td>Yes</td>
<td>30, 60, 90</td>
</tr>
<tr>
<td>SRD</td>
<td>Sequential Residual Design</td>
<td>Yes</td>
<td>30, 60, 90</td>
</tr>
</tbody>
</table>

The designs were chosen to establish which design objectives are best suited to provide the most accurate DACE model. The design based on randomly selected points (RND) consists of randomly chosen points from a uniform distribution where points outside the constraint space are rejected (see Figure 4.5a). The number of design points is satisfied by iteratively generating new designs where the amount of points in the square domain is adjusted by a ratio of the required number of sample points to the current number of sample points inside the sampling domain. This is repeated until the current number of points equal the required number of points.
McKay et al. [1979] introduced the Latin Hypercube Design (LHD) as an improvement over random sampling for input variables to computer code (see Figure 4.5b). It ensures that the design is space-filling to a certain extent by dividing the sample space into $n_{\text{samp}}$ rows and columns and requiring that there is only one sample point in each row and column. The space-filling measure of the design can be further improved by generating a series of Latin hypercubes and choosing the one which maximizes the minimum euclidean distance between points. This is known as the maximin criterion [Santner et al., 2003].

The Uniform Design in Cartesian coordinates (UDC) is a full factorial design in Cartesian coordinates with the points outside of the constraint space rejected (see Figure 4.5c). Therefore the number of sample points can only assume certain discrete values and the resolution is chosen to minimize the difference between the required number of sample points and that available. The Uniform Design in Polar coordinates (UDP) is a full factorial design as well (see Figure 4.5d), but in polar coordinates, and therefore the number of points are chosen as $(\text{round}(\sqrt{n_{\text{samp}}}))^2$. Due to the points becoming more spread out as the radius increases, more are concentrated in the center region which results in points being roughly normally distributed in the Cartesian coordinate system (see Figure 4.4).

The Uniform Triangulated Mesh (UTM) makes use of an unstructured mesh generator [Persson and Strang, 2004] which utilizes an iterative procedure to
Chapter 4. Preliminary bubble flow model investigation

triangulate the data with Delaunay triangulation together with solving for the position of the points by treating the mesh as a truss and solving for a force equilibrium (see Figure 4.5e). This leads to approximately equilateral triangles, resulting in a fairly evenly spread out design which is adaptable to complex geometries. The meshing scheme is applicable to n-dimensions but is largely untested for higher than 3 dimensions.

The Critical Point Design (CPD) is a novel sampling design introduced in this study which makes use of the high resolution data available to compute the first and second order derivatives of the model with the central difference formula. The first derivative is used to determine where local extrema in both directions in the data occur. These extrema may occur along ridges in the data and therefore may include many points. The magnitude of the second order derivative is then used to rank the importance of these extrema in order to identify the regions where the gradients are steepest. The required number of sample points can then be picked as the highest ranked points. Since these gradients tend to be steepest in certain regions, the top ranked points tend to be clustered together which is not good for the space-filling requirement of DACE models. Therefore a minimum distance criterion is also incorporated which starts at the highest ranked point and adds a penalty value to all points not conforming to its minimum distance criterion. This procedure is repeated as it moves through all the points, ensuring that points are spread out to the degree required. The CPD-L design represents a low value where the points are closer together whereas the CPD-H design uses a high minimum distance (Figures 4.5f and 4.5g).

Sequential experimental designs are an efficient alternative to fixed-point designs (all the above designs) and allow the DACE model to be optimised to a certain criterion by sequentially adding sampling points accordingly. Often the goal is to find the global optimum and an efficient improvement algorithm by Jones et al. [1998] has been shown to produce good results. More recently Lam [2008] introduced the Expected Improvement Criterion for Global Fit (EIGF) which was shown to perform well compared to other criteria. The use of EIGF has also been demonstrated by van Helden et al. [2012] with application to microkinetic analysis. These sequential design criteria are for the selection of a new point under
the absence of data, however since high resolution data is available, it is possible to optimise the accuracy of the overall fit according to the mean squared error of the DACE predictor, which is the criterion used for the Sequential Residual Design (SRD) in this study.

The SRD is the most computationally expensive design. Initially only a few points are present on which a DACE fit is performed (the optimisation process uses higher stopping criteria otherwise the process would be too computationally expensive), a point is then sequentially added at the location where the absolute residual is maximum (see Figure 4.5h). This is repeated until the desired amount of points are obtained. Since it is computationally demanding, it will only be examined with the powered exponential correlation function (Eq. (2.41)). This method can also be used in combination with other designs where the initial design is augmented with a number of sequential points, which accounts for features the original design criterion do not take account of. For this investigation this has been examined with the UDC, UDP, UTM and CPD-H designs, with a third of the points sequentially added.
Figure 4.5: Examples of the sampling designs being evaluated.
Chapter 4. Preliminary bubble flow model investigation

4.5 Results and Discussion

The aim of the work presented in this chapter is assessing the performance of the DACE modelling approach for different correlation functions and sampling designs presented in Sections 4.3.1 and 4.4 respectively, to the numerically generated velocity fields around a bubble within the operating range \( Re \leq 270 \). Since the optimisation of the correlation parameters can be computationally expensive, only the primary component of the velocity field is considered at five Reynolds numbers, i.e., at \( Re = 0.1, 15, 75, 135 \) and 270, for this preliminary investigation. The velocity fields are generated as discussed in Section 4.2, with the contours of these fields depicted in Figure 4.6. Key features of these fields is discussed below.

The velocity field for \( Re = 0.1 \) consists of smooth features which are symmetrical across the \( y = 0 \) line. As the Reynolds number increases to 15, the symmetry across \( y = 0 \) is lost and a tail feature begins to develop. At \( Re = 75 \), the flow features concentrate into smaller areas in the domain and become steeper. The transition from \( Re = 75 \) to 270 is characterized by further increases in the steepness of the gradients as the convection terms (see Eq. (4.1)) become more prominent. At higher Reynolds numbers the shape of the bubble changes while the flow becomes unsteady and the tail will begin to oscillate, resulting in more complex flow structures.

When summarizing the high resolution data such as in this case the sample points could be viewed as parameters to the DACE model and therefore it is favourable to summarize the data into as few sample points as possible. For this examination 3 levels, i.e., 30, 60 and 90, for the number of samples in the design \( (n_{samp}) \) are evaluated. Before commencing with the sampling designs and correlation functions, the estimation of the correlation parameters is to be considered.

4.5.1 Estimation Criteria

As mentioned in section 4.3.2 the residual with respect to the high resolution data can be used to optimise the correlation function parameters instead of using the MLE. This is evaluated by comparing the results from the different estimation
Figure 4.6: Scaled $\eta$-velocity contours for different Reynolds numbers, the blue tones denote higher relative velocities while the red represent the lower flow rates
methods for the five surfaces using a UDC design with 84 sample points. In order to prevent bias towards the residual criterion, the error comparison was performed on a grid of 91,055 points.

Table 4.2: Comparison of the maximum likelihood (MLE) and residual based parameter estimation criteria

<table>
<thead>
<tr>
<th>Method</th>
<th>Re = 0.1</th>
<th>Re = 15</th>
<th>Re = 75</th>
<th>Re = 135</th>
<th>Re = 270</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLE</td>
<td>6.91e-12</td>
<td>1.29e-05</td>
<td>2.45e-04</td>
<td>6.55e-04</td>
<td>2.10e-03</td>
</tr>
<tr>
<td>Residual</td>
<td>3.75e-13</td>
<td>1.24e-07</td>
<td>8.11e-06</td>
<td>4.65e-05</td>
<td>2.87e-04</td>
</tr>
</tbody>
</table>

It is seen from Table 4.2 that in all cases, minimizing the sum of squares of the residual produced much better results. It is therefore concluded that this method will be the most efficient for the data under consideration.

4.5.2 Investigation

The different DACE fits are compared on the basis of the mean squared error of the prediction at the original data points. All the results are tabulated in Tables B.1 to B.6 in Appendix B of this text. Some of the results for the MSE as a function of the $n_{\text{samp}}$ for the different designs are depicted in Figure 4.7 and 4.8. Examples of good fits for each surface is also depicted together with their designs in Figure 4.9.
Chapter 4. Preliminary bubble flow model investigation

Figure 4.7: Designs and \( n_{\text{samp}} \) compared based upon the MSE for different surfaces and correlation functions at \( Re = 0.1 \) and 75

(a) \( Re = 0.1, \ corr = \text{EXP-C} \)

(b) \( Re = 75, \ corr = \text{Matérn} \)
Chapter 4. Preliminary bubble flow model investigation

Figure 4.8: Designs and $n_{\text{samp}}$ compared based upon the MSE for different surfaces and correlation functions at $Re = 270$

(a) Re = 270, corr = EXP-C

(b) Re = 270, corr = EXP, designs = SRD
Figure 4.9: Examples of good fits; marker dots indicate sample points.
4.5.3 Discussion

4.5.3.1 Correlation Function

The general powered exponential correlation (EXP) was the most computationally efficient to optimise, as evident from Table 4.3, and the least prone to producing ill-conditioned covariance matrices. It does not require assumptions about the data and can represent different types of behaviours due to its flexible form.

The Matern correlation function produced the largest prediction errors for all the different designs and surfaces evaluated. This may be a result of the correlation function being prone to producing ill-conditioned covariance matrices, which results in “NaN” being passed to the optimisation scheme for certain combinations of correlation function parameters. This influences the optimisation scheme to move away from potential regions of global minima and therefore results in difficulty in finding the global minima. The Matern correlation function is therefore not recommended for use with computer experiments of CFD code since the increased computational effort does not yield a better fit.

The modified exponential correlation, EXP-C, consistently produced the lowest MSE’s. It shows that the behaviour of the data is not the same throughout the domain and varies with distance to the center of the bubble. Therefore, including this feature renders the correlation function more flexible. However, it may produce more ill-conditioned covariance matrices than the EXP correlation and was the most expensive to optimise as shown in Table 4.3. The increased computational expense could partly be attributed to the extra parameter, $s$, that is estimated, however, this can be justified by the improved accuracy of the fits. It should be noted that the way the point of interest in the EXP-C correlation function is incorporated, i.e., by modifying the $\Theta$’s, does not impact the conditioning of the covariance matrix as negatively as directly including the point of interest in the correlation equation.

It is noted that the computational expense for constructing the DACE models can be significant (in the range of 1 to 40 minutes depending on the correlation function and number of sample points, reported in Table 4.3). The approach fol-
Table 4.3: Generation times of DACE models with the EXP, EXP-C and Matérn correlation functions with varying number of sample points, $n_{samp}$. The times are averaged with respect to the Sampling Design and given in minutes.

<table>
<thead>
<tr>
<th>$n_{samp}$</th>
<th>EXP</th>
<th>EXP-C</th>
<th>Matérn</th>
<th>SRD (EXP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>1.2</td>
<td>2.3</td>
<td>7.3</td>
<td>5.8</td>
</tr>
<tr>
<td>60</td>
<td>2.3</td>
<td>29.3</td>
<td>18.1</td>
<td>20.7</td>
</tr>
<tr>
<td>90</td>
<td>2.6</td>
<td>36.0</td>
<td>31.0</td>
<td>42.1</td>
</tr>
</tbody>
</table>

allowed in this study to reduce the overall time of computation was to run multiple fits simultaneously on a multi-core processor. However, when considering a larger number fits in follow on studies (e.g., modelling non-spherical bubbles), taking advantage of parallel processing could be advantageous. The major contributor of computational expense is the optimisation of the correlation function parameters, where computation of the correlation between the sample points and the evaluation points takes the most computing time due to the large number of simple calculations. Since these calculations are independent of each other, it may be useful to divide these calculations into segments to be carried out by individual processors to take advantage of parallel CPU architecture. Furthermore, it may also be possible to perform these calculations on General Purpose Graphics Processing Units (GPGPU) (e.g., [Yang et al., 2012]). A cluster of computing CPU’s or GPGPU’s would be appropriate for a large number of fits. It follows that different options exist when considering large amounts of data to compute the DACE fits in a practical time frame.

4.5.3.2 Sampling Designs

The LHD was found to generally perform slightly better than the RND although this was not always the case. It would be preferred over random points since it guarantees some degree of uniformity in univariate dimensions, whereas in some cases randomly chosen points can be very close together resulting in ill-conditioned covariance matrices.

The UDC performed reasonably well for the $Re = 0.1$ and 15 surfaces (Tables
Chapter 4. Preliminary bubble flow model investigation

B.1 and B.2), but performed poorly with \( n_{\text{samp}} = 56 \), and below average with \( n_{\text{samp}} = 84 \) for the \( Re = 75, 135 \) and 270 surfaces (Tables B.3, B.4 and B.5). This was due to the spacing of the points which resulted in no points directly on the region where the tail feature is present. Therefore certain design criteria might be inefficient to describe certain features in the data, even though the design is uniform in some sense. Alternatively a maximin or sequential design criterion may be employed together with the uniformity criterion for constructing an improved design. Specifically, from Figure 4.8b it can be observed that the UDC+SRD performs reasonably well, which illustrates how the addition of another criterion can vastly improve the DACE model.

In contrast to the UDC, the UDP places points directly on the tail feature where the high residuals for these surfaces occur, and therefore yielded a smaller MSE. The UDP also inherently places more points close to its reference point while maintaining some uniform scatter of points, which was advantageous for the data investigated. However, it must be noted that it also performed well for the \( Re = 0.1 \) case (see Figure 4.7a) where no tail feature is present, which implies that this design could be useful for any data which has some point of interest or region where the data is most non-linear.

The UTM resulted in excellent fits for \( Re = 0.1 \) and comparable fits for the other surfaces. This again is due to the non-linear tail feature which dominates the errors for those surfaces. It did however perform better than the UDC in all cases which makes it a good choice for non-rectangular geometries in 2 and 3 dimensions. Sophisticated meshing algorithms are freely available which spread points out evenly subject to very complex geometries [e.g, Persson and Strang, 2004; Schöberl, 1997].

The CPD performed best when a high minimum distance was specified between the points. Therefore, in addition to selecting points in the critical areas, these points should be subjected to some space-filling criterion in order to obtain accurate DACE models. A design whose only criterion is to spread out points can better represent the data than one where points are clustered together, even when a good criterion is used. The consistently best fixed point design was found as the one which identifies critical regions and then places the points inside based on
a maximum minimum distance which the number of samples would allow. The CPD-H combination with the EXP-C correlation function resulted in excellent fits and produced an MSE which was on average 8 times smaller than the other combinations. The SRD designs performed well (Table B.6), with the UTM+SRD design having consistently produced the lowest mean squared errors. It can be concluded that a design which aims to spread out points evenly, in combination with a sequential design criterion, produces the most accurate DACE models. Even the UDC which performed poorly for higher Reynolds numbers, performed even better than the UDP+SRD for Re = 270, since it has better space-filling properties than the UDP, whose design points are distributed towards the center (see Figure 4.4). Therefore it can be concluded that a design that is aimed at filling the design space would be the preferred starting design for a sequential strategy. Furthermore, it is shown that the rate of improvement from 60 to 90 points is higher with the sequential addition of points compared to the designs based on a single criterion.

4.6 Conclusion

The development of the BCM simulation approach requires accurate approximations of the micro-flow field around a bubble. For this purpose, a DACE approach has been evaluated to summarize the high resolution $y$-velocity data resulting from the numerical simulation of the Navier-Stokes equations with at least 3 orders of magnitude less overall parameters. Since high resolution data is available, the covariance function is optimised subject to the mean squared error of the prediction which is shown to yield more accurate fits than the typically applied maximum likelihood estimation. This also provided an opportunity to evaluate the performance of different sampling criteria and covariance correlation functions in an assessable manner.

The powered exponential correlation proved to be the most computationally efficient to optimise. A modified powered exponential function introduced here, which is distance dependent to the centre of the bubble, yielded the best overall
results. Due to the improvement in model accuracy, this correlation function has the potential to be successfully applied to a wider suite of industrial modelling problems. Seven different design of experiment approaches have been evaluated for developing DACE models. It is recommended that a design with good space-filling properties be used for performing computer experiments. Combining design criteria can vastly improve the accuracy of the final design as shown with the UDC+SRD case. Specifically, compound or sequential design strategies can be used to add design points where the model is highly non-linear with steep gradients. The critical point design (CPD) has been introduced and shown to be superior compared to the other designs for many of the cases evaluated. Specifically, the CPD combined with a space-filling criterion was shown to be the best non-sequential design.

This research shows how the velocity field over a fluid sphere can effectively be summarized using the DACE approach. It has been found that accurate approximations are possible through the choice of sampling design strategy and correlation function. Specifically, the application of a location dependent correlation function together a gradient based sample point selection with a space-filling criterion yields accurate models for approximating the velocity fields considered. These results show that it is possible to construct the stage 1 models at various Reynolds numbers for the development of the BCM. The following chapter will focus on the application of analytical models to reduce the number of parameters and additional BCM modelling strategies.
Chapter 5

Semi-analytical bubble flow model development

This chapter reports the integration of analytical models, to account for some of the flow features of the first stage BCM, with statistical models. The analytical solutions are based on the axisymmetric treatment of the Navier-Stokes equations that describes the velocity vector field with respect to radial and angular velocities (Section 5.1.1). Since the analytical models cannot account for all the flow features (due to simplifying assumptions), two different statistical approaches are evaluated to approximate the resulting deviations (Section 5.2.2 and 5.2.3). The final semi-analytical models are evaluated and compared based on accuracy and number of parameters for both the radial and angular velocities in Section 5.3. This chapter concludes the stage one development of the BCM with accurate semi-analytical flow models.
Chapter 5. Semi-analytical bubble flow model investigation

5.1 Modelling flow over a fluid sphere

5.1.1 Simplified analytical solutions

Analytical solutions to the steady state incompressible Navier-Stokes equations (see Eq. 2.3 and 4.1) provide a potentially useful starting point for the development of the BCM, since they are based in the conservation fundamentals of the governing equations and capture useful features of the flow structure. Solutions are possible through simplifying assumptions, such as zero advective terms (i.e., creeping flow), or zero viscosity (i.e., potential flow), rendering Eq. 2.3 and 4.1, analytically solvable (simplifications to the Navier-Stokes equations are discussed in Section 2.2 in the literature review chapter).

\[ \nabla^* \mathbf{u}^* = 0 \]  
\[ \left( \mathbf{u}^* \cdot \nabla^* \right) \mathbf{u}^* = -\nabla^* P^* + \frac{1}{Re} \nabla^2 \mathbf{u}^* \]  

The creeping flow solution was derived by Stokes [1851] for flow over fixed sphere and is valid at the theoretical limit of \( Re \to 0 \). Assuming axisymmetric flow and formulating the Navier-Stokes equations in terms of the Stokes stream function (\( \psi \)) in spherical coordinates, simplifies the problem considerably. The radial and angular components, \( r \) and \( \theta \), are centered around the bubble. The corresponding radial and angular velocity components, \( u_r \) and \( u_\theta \), are related to \( \psi \) through Eq. 5.1 and 5.2, resulting in mass continuity being unconditionally satisfied. Following the solution strategy presented by Slattery [1999], \( \psi \) is proposed as a fourth order polynomial whose coefficients are obtained through the substitution of the boundary conditions. Applying the zero-shear-stress boundary condition (Eq. 5.3 to 5.5, where \( u_\infty \) represents the free stream velocity and is related to the relative bubble velocity through \( u_\infty = -u_{rel} \)), appropriate for clean bubbles [Clift et al., 1978], \( \psi \) can be obtained, which upon differentiation yields the solutions for \( u_r \) and \( u_\theta \). These solutions, superscripted for creeping flow as \( u_r^c \) and \( u_\theta^c \), are
Chapter 5. *Semi-analytical bubble flow model investigation*

given in Eq. 5.6 and 5.7, and plotted as contour lines in Figure 5.1a and 5.1c respectively (the derivation of Eq. 5.6 and 5.7 is presented in Appendix A).

\[
\begin{align*}
\mathbf{u}_r &= \frac{1}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial \theta} \\
\mathbf{u}_\theta &= \frac{1}{r \sin(\theta)} \frac{\partial \psi}{\partial r} \\
\end{align*}
\]  

(5.1)

\[
\begin{align*}
\mathbf{u}_r|_{r\to\infty} &= u_\infty \cos(\theta) \\
\mathbf{u}_r|_{r=R} &= 0 \\
\frac{d\mathbf{u}_\theta|_{r=R}}{dr} &= 0 \\
\end{align*}
\]  

(5.3) (5.4) (5.5)

\[
\begin{align*}
\mathbf{u}_c^r &= u_\infty \left[ 1 - \frac{3}{4} \frac{R}{r} - \frac{1}{4} \left( \frac{R}{r} \right)^3 \right] \cos(\theta) \\
\mathbf{u}_c^\theta &= u_\infty \left[ 1 - \frac{3}{8} \frac{R}{r} + \frac{1}{8} \left( \frac{R}{r} \right)^3 \right] \sin(\theta) \\
\end{align*}
\]  

(5.6) (5.7)

Although zero viscosity fluids do not physically exist, the assumption (which applies in the limit of \(Re \to \infty\)) provides a reasonably good description of the velocity profile, except near the body and beyond the line of flow separation [Bird et al., 2002]. The potential flow solution is derived by defining velocity potential \(\Phi\), such that \(\mathbf{u} = -\nabla \Phi\). The zero-shear-stress boundary condition, is intrinsically satisfied by the inviscid assumption. For incompressible potential flows, \(\Phi\) satisfies Laplace’s equation which can be solved with the method of separation of variables [Slattery, 1999], and upon differentiation returns the potential flow velocity fields, \(\mathbf{u}_c^r\) and \(\mathbf{u}_c^\theta\), given in Eq. 5.8 and 5.9 and plotted in Figure 5.1b and 5.1d respectively.
Chapter 5. *Semi-analytical bubble flow model investigation*

\begin{align*}
    \mathbf{u}_p^\theta &= u_\infty \left[ -1 + \left( \frac{R}{r} \right)^3 \right] \cos(\theta) \quad (5.8) \\
    \mathbf{u}_p^r &= u_\infty \left[ 1 + \frac{1}{2} \left( \frac{R}{r} \right)^3 \right] \sin(\theta) \quad (5.9)
\end{align*}

Figure 5.1: Contours of analytical velocity fields. Here $x$ and $y$ denote the Cartesian spatial coordinates centered around the bubble; this is divided by the bubble radius, $R$, for dimensionless coordinates.
Chapter 5. *Semi-analytical bubble flow model investigation*

The solutions for both simplifying assumptions are simple algebraic expressions that allow for rapid numerical function evaluation. The velocity contours of the numerical solution of the complete Navier-Stokes equations (i.e., without simplifying assumptions) are depicted in Figure 5.2 for $Re = 270$. Upon comparison of the analytical solutions in Figure 5.1 with 5.2, it is evident that neither of the analytical solutions are able to capture the flow separation and wake features at the rear of the bubble, which are artefacts arising when $Re > 1$. This results in poor flow prediction from the analytical models at the rear of the bubble and incorrect hydrodynamic force calculation, thereby limiting the practical applicability of these solutions.

### 5.1.2 General numerical solutions

The combination of both convective and viscous terms in the Navier-Stokes equations requires the application of numerical methods to obtain a solution. Here the finite volume method together with the SIMPLE pressure-velocity coupling scheme [Pantankar, 1980] is applied to solve the axisymmetric Navier-Stokes equations to obtain numerical solutions for $u_r$ and $u_\theta$.

A grid resolution independent solution is obtained by solving the axisymmetric Navier-Stokes equations at $Re = 270$ on consecutively finer grids and calculating the force on the bubble. The force approaches a constant value at a resolution of 166816 cells which is taken as the grid independent solution. The resulting velocity vector fields produced on this grid is regarded as the true velocity field, $u_r^t$ and $u_\theta^t$, for each Reynolds number. The contours of $u_r^t$ and $u_\theta^t$ for $Re = 270$ are depicted in Figure 5.2.

The time required to evaluate the analytical models when compared to the iterative solution of $u_r^t$ and $u_\theta^t$ is negligible, however they are not capable of accounting for certain key flow features. For the rapid evaluation of the flow field around a bubble within a bubble column simulator, statistical models will subsequently be considered.
Chapter 5. Semi-analytical bubble flow model investigation

Figure 5.2: Velocity contours for the numerical solution of the axisymmetric Navier-Stokes equations at \( Re = 270 \).

5.2 Statistical approximations

5.2.1 Combined analytical models

The application of statistical modelling arises from an attempt to bridge the gap between the two extrema cases of the analytical solutions i.e., \( Re = 0 \) and \( Re = \infty \), by accounting for features occurring in the non-idealized flow regimes. Since the focus of the bubble column simulator under development is on high-speed computations, a semi-analytical model, expressed as simple algebraic formulations, would be justified over the solving of the non-linear Navier-Stokes equations.

As a first approximation to the velocity vector field, the creeping and potential flow analytical solutions presented in 5.1.1, are applied in a linear combination, where \( \mathbf{u}_r^{m,a} \) and \( \mathbf{u}_\theta^{m,a} \) represents the resulting models (see Eq. 5.10 and 5.11). The weights, \( [\eta_{r,1}, \eta_{r,2}] \) and \( [\eta_{\theta,1}, \eta_{\theta,2}] \), are obtained using linear least squares with respect to \( \mathbf{u}_r^c \) and \( \mathbf{u}_\theta^c \). It follows that these combined analytical models are functions of \( Re \), spatial position (\( x \)) and linear weight coefficients, such that \( \mathbf{u}_{r/\theta}^{m,a} \) can be written as \( \mathbf{u}_{r/\theta}^{m,a} = \mathbf{u}_{r/\theta}^{m,a}(Re, x, \eta) \). Since both analytical solutions are
symmetrical with respect to the front and the rear of the bubble (fore-and-aft symmetry), and most of the deviations occur at the rear, the weights are fitted to the frontal data i.e., \( y \geq 0 \).

\[
\begin{align*}
\mathbf{u}_r^{m,a} &= \eta_{r,1} \mathbf{u}_r^c + \eta_{r,2} \mathbf{u}_r^p \\
\mathbf{u}_\theta^{m,a} &= \eta_{\theta,1} \mathbf{u}_\theta^c + \eta_{\theta,2} \mathbf{u}_\theta^p
\end{align*}
\]  
(5.10)

(5.11)

The residuals, \( \mathbf{u}_{r}^{res} \) and \( \mathbf{u}_{\theta}^{res} \), are defined in Eq. 5.12 and 5.13 (see also Figure 5.4), and expressed as relative percentage errors, \( \mathbf{u}_{r}^{\%} \) and \( \mathbf{u}_{\theta}^{\%} \), in Eq. 5.14 and 5.15. The cumulative distribution of \( \mathbf{u}_{r}^{\%} \) and \( \mathbf{u}_{\theta}^{\%} \) at different \( Re \) (see Figure 5.3) gives an indication of the suitability of \( \mathbf{u}_{r}^{m,a} \) and \( \mathbf{u}_{\theta}^{m,a} \) and the deviation of the Navier-Stokes solution from the analytical solutions.

\[
\begin{align*}
\mathbf{u}_r^{res} &= \mathbf{u}_r^t - \mathbf{u}_r^{m,a} \\
\mathbf{u}_\theta^{res} &= \mathbf{u}_\theta^t - \mathbf{u}_\theta^{m,a} \\
\mathbf{u}_{r}^{\%} &= \frac{100 \cdot |\mathbf{u}_r^{res}|}{\max(\mathbf{u}_r^t) - \min(\mathbf{u}_r^t)} \\
\mathbf{u}_{\theta}^{\%} &= \frac{100 \cdot |\mathbf{u}_\theta^{res}|}{\max(\mathbf{u}_\theta^t) - \min(\mathbf{u}_\theta^t)}
\end{align*}
\]  
(5.12)

(5.13)

(5.14)

(5.15)
Figure 5.3: Cumulative distribution of $u_r^{\%e}$ and $u_\theta^{\%e}$. 
Chapter 5. *Semi-analytical bubble flow model investigation*

It is observed that both models produce reasonable approximations to the true model, yielding lower error distributions with increasing Reynolds numbers, i.e., from $Re = 15$ to 270, for both models (see Figure 5.3). As $Re$ is increased, the bubble wake becomes concentrated into a smaller spatial area, leading to the overall error distribution becoming smaller. The trend is however, reversed when comparing $Re = 15$ to 0.1 as the creeping flow approximation is approached, which follows expectation.

A comparison between the two velocity models, show $u^{\theta \epsilon}$ yielding lower error percentages. This is due to deviations from the analytical models being concentrated in a smaller area, as evident from the surface plot of the residuals in Figure 5.4. It is concluded that $u^{m,a}_{\theta}$ and $u^{m,a}_{\theta}$ present useful models that can accurately approximate large portions of the flow field, however, important features such as the bubble wake, cannot be represented and requires further modelling. Subsequently two different modelling strategies i.e., regression with empirical models (Section 5.2.2) and DACE models (Section 5.2.3) are evaluated for capturing the residuals $u^{\text{res}}_{r}$ and $u^{\text{res}}_{\theta}$.

### 5.2.2 Empirical modelling

This section deals with the fitting of the residual velocity surfaces, i.e., $u^{\text{res}}_{r}$ and $u^{\text{res}}_{\theta}$, by identifying key features in the data that can be approximated by simple functions. The radial velocity residual is treated first (Section 5.2.2.1) followed by the angular velocity residual (Section 5.2.2.2).

#### 5.2.2.1 Fitting of radial velocity residual

The residual of the radial velocity exhibits strong spatial dependence (as seen in Figure 5.4a), which could potentially be approximated if the appropriate functions are found. To allow for accurate fitting with simple models, it is proposed to discretise the domain into two regions to isolate the tail feature. The choice of domain discretisation and models must be applicable across the Reynolds operating range.
Chapter 5. Semi-analytical bubble flow model investigation

Figure 5.4: Residual surface plots at $Re = 135$.

It is observed that choosing a critical angle, $\theta_c$, based on the maximum of the residual i.e., Eq. 5.16, corresponds to the small peak at the rear of the bubble which isolates the Gaussian behaviour of the tail feature while the remainder
decays exponentially in the angular direction.

\[ \theta_c = \theta(\max[u_r^{\text{res}}(\theta, r)]) \] (5.16)

Since the peaks behind the sphere occur across the operating range, \( \theta_c \) serves as an useful discretiser for the purpose of the BCM. The trend is for \( \theta_c \) to decrease with increasing \( Re \) as the wake becomes thinner (see Figure 5.5).

**Region 1 (\( R_1 \))**

The definition of \( \theta_c \) allows the wake feature, which contains the highest concentration of residual, to be isolated and considered separately, thereby simplifying the problem. The region exhibits Gaussian behaviour in the angular direction, however, this behaviour is also radially dependent in a non-linear fashion. Therefore, the approach taken is to fit each radial shell of \( u_r^{\text{res}} \) with respect to \( \theta \) by interpolating the data onto a uniform polar grid, and looping over each radial shell. The data from each radial shell is smoothed such that numerical noise is removed (using locally weighted scatterplot smoothing [Cleveland, 1979]) and fitted to the model \( u_{r_{\text{m}, R_1}} \), given in Eq. 5.17. Non-linear least squares is used to obtain the model parameters \( A, B \) and \( C \), where the initial values are obtained from the result of the previous shell, resulting in minimal “jumps” in the values of the parameters, thereby yielding a smooth response of \( A, B \) and \( C \) with respect to \( r \).

\[ u_{r_{\text{m}, R_1}} = A \exp\left(\frac{(\theta - \pi)^2}{B}\right) + C \] (5.17)

The empirical relation proposed in Eq. 5.17, presents a good approximation to the radial shells of the tail feature as illustrated in Figure 5.6. To describe the variation of the Eq. 5.17 parameters (\( A, B \) and \( C \)) with respect to \( r \), each of parameters is modelled as a function of \( r \). It is observed that all exhibit exponential behaviour (depicted in Figures 5.7 to 5.9), with \( A \) and \( C \) having characteristics of the sum of exponentials and \( B \), the form of exponential decay. This is con-
Chapter 5. *Semi-analytical bubble flow model investigation*

Figure 5.5: Contours of $|\mathbf{u}_r^{\text{res}}|/u_\infty$, illustrating the change of $\theta_c$ w.r.t. Reynolds number. $R_1$ and $R_2$ here denote region 1 and region 2 for $\mathbf{u}_r^{\text{res}}$ respectively.

Confirmed with the evaluation of various curve fitting models, where Eq. 5.18 to 5.20 provides the best representation, with the least amount of parameters across the operating range (the empirical model parameters are collectively termed $\varphi$ with appropriate subscripts for each model).
Chapter 5. *Semi-analytical bubble flow model investigation*

The proposed models produce a reasonable fit to the data with low error propagation i.e., small errors in the parameter models do not result in large errors in the overall fit. This could be attributed to the exponential form of Eq. 5.17 which is less sensitive to its parameters than for example a high order polynomial model, which is highly sensitive to small changes in its parameters. Subsequently, Eq. 5.17 together with Eq. 5.18 to 5.20, presents a suitable model for $\mathbf{u}^\text{res,R1}$, based on accurate fits and relatively low error propagation of its parameters.

$$
A = \varphi_{a,1} \exp (-\varphi_{a,2} r) + \varphi_{a,3} \exp (-\varphi_{a,4} r) \tag{5.18}
$$

$$
B = \varphi_{b,1} \exp (-\varphi_{b,2} r) + \varphi_{b,3} \tag{5.19}
$$

$$
C = \varphi_{c,1} \exp (-\varphi_{c,2} r^2) + \varphi_{c,3} \exp (-\varphi_{c,4} r^2) + \varphi_{c,5} \tag{5.20}
$$

Figure 5.6: $R^2$ statistic for Eq. 5.17 with respect to radial shells $(r/R)$ of $\mathbf{u}^\text{res}$ at $Re = 270$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.6.png}
\caption{$R^2$ statistic for Eq. 5.17 with respect to radial shells $(r/R)$ of $\mathbf{u}^\text{res}$ at $Re = 270$.}
\end{figure}
Chapter 5. *Semi-analytical bubble flow model investigation*

Figure 5.7: $u_r^{m,R_1}$ region 1 parameter fitting for $Re = 15$.

Figure 5.8: $u_r^{m,R_1}$ region 1 parameter fitting for $Re = 135$.

**Region 2 ($R_2$)**

The data in region 2 exhibits an overall decaying trend in the $\theta$ direction. Deviations from this trend constitutes relatively low residual values which does not
justify the use of models involving more parameters. Subsequently, the model used is the exponential decay of $u_{r}^{m,R1}$ at $\theta = \theta_c$, that ensures continuity between the region 1 and 2 models, $u_{r}^{m,R1}$ and $u_{r}^{m,R2}$. The form of exponential decay was determined by examining functions of both $\theta$ and $r$. It was found that a function of only $\theta$ and two regression parameters, $\varphi_{d,1}$ and $\varphi_{d,2}$, approximates $u_{r}^{\text{res}}$ in region 2 with the lowest error (see 5.21). Surfaces of $u_{r}^{\text{res},R2}$ in region 2 and $u_{r}^{m,R2}$ are plotted in 5.10.

$$u_{r}^{m,R2} = u_{r}^{m,R1}|_{\theta = \theta_c} \exp \left( - (\varphi_{d,1}(\theta_c - \theta)^2 + \varphi_{d,2}(\theta_c - \theta)) \right) \quad (5.21)$$

### 5.2.2.2 Fitting of the angular velocity residual

From the contour plots of $u_{r}^{\text{res}}$ illustrated in 5.11, it is seen that the residual is mostly concentrated in the direct vicinity to the rear of the bubble, from where it decays radially. Furthermore, $u_{r}^{\text{res}}$ is a maximum at the surface of the bubble. A resulting strategy is to approximate $u_{r}^{\text{res}}$ at $r = R$ with a $\theta$ dependant model,
Chapter 5. Semi-analytical bubble flow model investigation

Figure 5.10: Scaled surface plots of region 2 radial velocity residual ($u_{r}^{\text{res},R2}$) and approximation ($u_{r}^{m,R2}$) at $Re = 270$. The numerical noise in plot (a) is due to very small numerical errors in the CFD simulation.

$u_{r}^{m,R1}$, followed by the fitting of the radial decay with a second model, $u_{r}^{m,R2}$. Thereby, with respect to $u_{r}^{\text{res}}$, $R_1$ refers to the region at the surface of the bubble ($r = R$), while $R_2$ refers to the rest of the domain.

The shape of the data at the bubble surface, $u_{r}^{\text{res}}|_{r=R}$, is Gaussian, however, it is not symmetric about the peak, as seen in 5.12. The multiplication of a Gaussian model with an error function, i.e., Eq. 5.22, was therefore found to fit the data accurately and is used for this purpose.

$$u_{r}^{m,R1} = -\varphi_{r,1}\left(\exp(-\varphi_{r,2}(\theta - \varphi_{r,3})^2) + \varphi_{r,4}\theta\right)erf(-\varphi_{r,5}(\theta - \varphi_{r,3})) \quad (5.22)$$

With the accurate fit of $u_{r}^{\text{res}}|_{r=R}$ with $u_{r}^{m,R1}$, the residual decay from the bubble surface can be approximated. This decay was found to behave exponentially with both radial and angular dependence, where Eq. 5.23 was found to describe the behaviour.
Figure 5.11: Contours of $u_\theta^{\text{res}}/u_\infty$ with varying Reynolds number.

\begin{align}
\mathbf{u}_\theta^{m,R2} = u_\theta^{m,R1}(\theta) \exp \left( - \varphi_{f,1}(r - R) + \varphi_{f,2}(r - R)\theta \right)
\end{align}

(5.23)
5.2.3 Design and Analysis of Computer Experiments

The DACE methodology, evaluated in Chapter 4, is considered here for summarizing $u_r^{\text{res}}$ and $u_\theta^{\text{res}}$ to a few critical points. Subsequently, a set of sample points, $S$, is selected from the grid, and the corresponding responses, $Y_s$, are correlated to one another through a distance dependent correlation function ($\mathcal{R}$). The DACE strategy therefore involves modelling the correlation between a set of critical sample points and the prediction points, as opposed to the empirical strategy which entails proposing functional forms which approximate key features in the data. The powered exponential correlation function, also referred to as the Kriging distance function [Jones et al., 1998], is the exponential function of the
sum of the weighted absolute distances, where $S_{ik}$ is the $i$-th sample point for the $k$-th dimension, for each of the $n_d$ spatial dimensions (see Eq. 5.24 and 5.25, the distance function is referred to as $D$ in this chapter for convenient comparison). The weighting parameters, $\Theta$’s and $p$, are estimated through optimisation with respect to the maximum likelihood estimation [Sacks et al., 1989], however, with dense data available, it has been found from the previous chapter that the mean squared error with respect to the available data results in better approximations, which will be used to estimate the parameters for this investigation. The reader is referred to the previous chapter or Coetzee et al. [2012a] for a stepwise numerical procedure for constructing the DACE model and estimating its parameters.

$$D = \sum_{k=1}^{n_d} \Theta_k |S_{i,k} - S_{j,k}|^p \quad (5.24)$$
$$R = \exp(-D) \quad (5.25)$$

It follows from Figure 5.4 that the data, $u_{r}^{\text{res}}$ and $u_{b}^{\text{res}}$, is distributed in identifiable regions, which implies very strong correlation between the points in the low residual regions and weaker correlation in the higher residual regions. Since the powered exponential correlation function is only dependent on the distance between points, it would be beneficial for the correlation model to exhibit some regional dependence. In Chapter 4, a modified powered exponential function was presented which was found to improve the accuracy of the fits (Eq. 5.26 to 5.30). This correlation function is of the form applied to dual response surface optimisation problems [Coetzer et al., 2008] and uses a desirability function, $m(w)$ related to some point of interest $x_c$. The point of interest is chosen as the centre of the bubble, the activity parameter set as an optimisation variable and the weighting parameter as $\lambda = 0.5$. 
Chapter 5. *Semi-analytical bubble flow model investigation*

\[ D^* = \sum_{k=1}^{n_d} \Theta_k^* |S_{i,k} - S_{j,k}|^p \]  
(5.26)

\[ \Theta_k^* = \Theta_k + \Theta_{k,1} m(w) \]  
(5.27)

\[ m(w) = \frac{\exp(s) - \exp(s|w|)}{\exp(s) - 1} \]  
(5.28)

\[ w = \lambda \sum_{k=1}^{n_d} \frac{(S_{i,k} - x_{c,k})^2}{(S_{\text{max},k} - S_{\text{min},k})^2} + (1 - \lambda) \sum_{k=1}^{n_d} \frac{(S_{j,k} - x_{c,k})^2}{(S_{\text{max},k} - S_{\text{min},k})^2} \]  
(5.29)

\[ \mathcal{R} = \exp(-D^*) \]  
(5.30)

A further modification to the powered exponential function is introduced in this chapter i.e., the product of the weighted distances (Eq. 5.24) with a series of error functions, which serves the purpose of demarcating a local zone with distinct spatial dependence. Two error functions, of the form Eq. 5.31, are multiplied for each dimension, i.e., one for the lower (\( \delta_{\text{min}} \)) and one for the upper limit (\( \delta_{\text{max}} \)), to define a zone enclosed by the domain. This concept is illustrated for one dimension in Figure 5.13. The product of the error functions (Eq. 5.32) results in a value between 0 and 1 which can be multiplied with the sum of the weighted distances inside the exponential function, defining the modified correlation function (Eq. 5.33). The corresponding parameters, \( \omega \)'s and \( \delta \)'s, can be optimised together with the \( \Theta \)'s and \( p \), such that the shape and location of the zone is optimal to the data being fitted. Furthermore, it is possible to account for more zones and apply to higher dimensions, however, the number of parameters to be estimated will increase accordingly. For this study two \( \omega \)'s (one for each dimension) and three \( \delta \)'s (two for the y-axis and only one for the x-axis due to symmetry at \( x = 0 \)) will be optimised.
Chapter 5. Semi-analytical bubble flow model investigation

\[ \ell_{\delta,k} = 0.5 \left( \text{erf} \left( \omega \left( 0.5 (S_{i,k} + S_{j,k}) - \delta \right) \right) + 1 \right) \]  
(5.31)

\[ L = 1 - \prod_{k=1}^{n_d} \ell_{\delta_{min,k}} (1 - \ell_{\delta_{max,k}}) \]  
(5.32)

\[ \Re = \exp(-LD) \]  
(5.33)

Figure 5.13: Spatial dependence weighting function \( L \) (Eq. 5.32).

The choice of sample points, \( S \), significantly influences the accuracy of the fit. For this investigation a Critical Point Design (CPD) is used, which was found from Chapter 4 to provide the best fits with the smallest number of sample points using similar data. The CPD is based on turning points in the data which are ranked according to the absolute value of their second order spatial derivative. Since points tend to be clustered together, a minimum distance criterion, \( \text{min}_{d} \), is implemented to spread the design points to a specified degree, which provides space filling functionality to the design. For the treatment of the symmetrical data, the turning points are based upon the data projected onto a full 2 dimensional grid, such that the turning points falling on the \( x = 0 \) axis can be determined. Furthermore, the points on the positive \( x \)-axis are mirrored onto the negative \( x \)-
axis, however the mirrored points are not considered as additional parameters and therefore not counted for the number of samples, \( n_{\text{samp}} \). The sampling designs for a low and high \( \min_d \) for the same data is illustrated in Figure 5.14.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5_14.png}
\caption{Resulting sample designs, \( S \), for \( u_{r_{\text{res}}} \) at \( \text{Re} = 270 \) with \( n_{\text{samp}} = 25 \).}
\end{figure}

The DACE model includes the general least squares solution of a regression model (Eq. 2.37). This regression is, however, based on the general least squares solution of the sample points and the sample points selection is based on where they represent the residual best. Therefore, the combination of the analytical models do not present a good DACE regression model, since the least squares solution at the sample points result in poor fits. A resulting strategy is to fit the analytical models to the data minus the DACE model. This strategy is carried out iteratively where the DACE model is fitted to the new residual value until the best combination of analytical and DACE models is obtained.

## 5.3 Results

The results from the DACE model are discussed first, followed by a comparison with the empirical model. At the outset, the different correlation functions, i.e., Eq. 5.25, 5.30 and 5.33 are evaluated. Due to the iterative nature of the optimisation scheme described in Section 5.2.3, the estimation of the DACE parameters
is computationally expensive and therefore only 6 discrete Reynolds numbers i.e., $Re = [0.1, 15, 75, 135, 195, 270]$, were chosen for the evaluation with $\min_d = 0.35$ and $n_{samp} = 25$. For the radial velocity residual, the modified correlations produced significantly lower mean squared errors, with $\exp(-LD)$ resulting in the lowest MSE for 4 of the 6 Reynolds numbers evaluated (Figure 5.15a). With the angular velocity residual, the $\exp(-LD)$ correlation resulted in the lowest MSE for all the Reynolds numbers with a significant improvement on the other two correlation functions evaluated (Figure 5.15b). It can be concluded that a correlation function with some location dependence would be preferred when the data is concentrated in specific regions. Furthermore, the $\exp(-LD)$ correlation delivered the best overall results and is therefore used in the subsequent evaluations.

To quantify the influence of the resolution of the grids used during the model construction on the accuracy of the fits, the empirical and DACE models are evaluated at three different grid sizes, i.e., $n_{grid} = [22500, 40000, 62500]$ points. The comparison was then made on a new grid of $n_{grid} = 50000$. The average standard error for the three different grid sizes across discrete Reynolds numbers of 0.1 to 270 with increments of 15, was found to be 0.34% and 0.10% for $u_r^{res}$ and $u_{\theta}^{res}$ respectively, using the empirical model. Similarly, the different grid sizes had no significant effect on the DACE model and it can therefore be concluded that grid resolution has no significant influence on the fit of the models in the size range considered and subsequent fits are based on grids with $n_{grid} = 40000$.

With the correlation function and grid resolution established, the parameters to the DACE model, $\min_d$ and $n_{samp}$, together with the Reynolds number were evaluated using a full factorial design. The levels for these variables are summarized in Table 5.1, which results in 72 fits for each of the velocity residual fields.

### Table 5.1: Variables with corresponding levels for the DACE model evaluation

<table>
<thead>
<tr>
<th>Variable</th>
<th>Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\min_d$</td>
<td>0.15, 0.25, 0.35, 0.45</td>
</tr>
<tr>
<td>$n_{samp}$</td>
<td>20, 30, 40</td>
</tr>
<tr>
<td>$Re$</td>
<td>0.1, 15, 75, 135, 195, 270</td>
</tr>
</tbody>
</table>
The results were compared by generating the model of each fit on a new grid with $n_{\text{grid}} = 50000$. The subsequent mean squared errors with the CFD generated output, $u^{res}_{\|}$ and $u^{res}_{\theta}$, could then be compared in an unbiased fashion. An analysis of variance of the parameters (Table 5.2 and 5.3) reveals the most significant
effect as $Re$. For $u_{\text{res}}^r$, the second biggest effect was $n_{\text{samp}}$, while $min_d$ was found to be the second biggest effect for $u_{\theta}^\text{res}$. The relative importance of $min_d$ for $u_{\theta}^\text{res}$ could be explained by the residual being concentrated in a smaller area. The corresponding levels of the best DACE models from the factorial evaluation is summarized in Table 5.4.

Table 5.2: Analysis of Variance for levels of DACE parameters for approximating $u_{\text{res}}^r$

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum Sq.</th>
<th>d.f.</th>
<th>Mean Sq.</th>
<th>F-ratio</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$min_d$</td>
<td>1.89795e-13</td>
<td>3</td>
<td>6.32649e-14</td>
<td>1.01</td>
<td>0.4001</td>
</tr>
<tr>
<td>$n_{\text{samp}}$</td>
<td>2.00005e-12</td>
<td>2</td>
<td>1.00003e-12</td>
<td>16.03</td>
<td>0</td>
</tr>
<tr>
<td>$Re$</td>
<td>1.02916e-11</td>
<td>5</td>
<td>2.05832e-12</td>
<td>33</td>
<td>0</td>
</tr>
<tr>
<td>$min_d*n_{\text{samp}}$</td>
<td>4.43735e-13</td>
<td>6</td>
<td>7.39559e-14</td>
<td>1.19</td>
<td>0.3404</td>
</tr>
<tr>
<td>$min_d*Re$</td>
<td>1.49595e-12</td>
<td>15</td>
<td>9.97302e-14</td>
<td>1.6</td>
<td>0.1334</td>
</tr>
<tr>
<td>$n_{\text{samp}}*Re$</td>
<td>2.52905e-13</td>
<td>10</td>
<td>2.52905e-13</td>
<td>4.05</td>
<td>0.0014</td>
</tr>
<tr>
<td>Error</td>
<td>1.87111e-12</td>
<td>30</td>
<td>6.23702e-14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.88213e-11</td>
<td>71</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.3: Analysis of Variance for levels of DACE parameters for approximating $u_{\theta}^\text{res}$

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum Sq.</th>
<th>d.f.</th>
<th>Mean Sq.</th>
<th>F-ratio</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$min_d$</td>
<td>1.41683e-11</td>
<td>3</td>
<td>4.72277e-12</td>
<td>32.13</td>
<td>0</td>
</tr>
<tr>
<td>$n_{\text{samp}}$</td>
<td>6.44119e-12</td>
<td>2</td>
<td>3.2206e-12</td>
<td>21.91</td>
<td>0</td>
</tr>
<tr>
<td>$Re$</td>
<td>1.50188e-10</td>
<td>5</td>
<td>3.00376e-11</td>
<td>204.35</td>
<td>0</td>
</tr>
<tr>
<td>$min_d*n_{\text{samp}}$</td>
<td>2.28572e-12</td>
<td>6</td>
<td>3.80953e-13</td>
<td>2.59</td>
<td>0.0383</td>
</tr>
<tr>
<td>$min_d*Re$</td>
<td>2.49633e-11</td>
<td>15</td>
<td>1.66422e-12</td>
<td>11.32</td>
<td>0</td>
</tr>
<tr>
<td>$n_{\text{samp}}*Re$</td>
<td>9.05888e-12</td>
<td>10</td>
<td>9.05888e-13</td>
<td>6.16</td>
<td>0</td>
</tr>
<tr>
<td>Error</td>
<td>4.40979e-12</td>
<td>30</td>
<td>1.46993e-13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>2.11515e-10</td>
<td>71</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The semi-analytical approximations resulting from both the empirical models and the DACE models with the lowest MSE’s, are depicted in Figure 5.16 and Table 5.5 and 5.6. In general, both approaches resulted in very accurate models of the velocity fields, with the DACE approach resulting in slightly lower MSE’s than the empirical strategy, especially for the angular velocity at lower Reynolds numbers. The choice between the two modelling approaches subsequently depends on the model requirements.
Chapter 5. *Semi-analytical bubble flow model investigation*

Table 5.4: Levels of DACE parameters resulting in lowest MSE for semi-analytical fit

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$u_r^{res}: n_{samp}$</th>
<th>$u_r^{res}: min_d$</th>
<th>$u_\theta^{res}: n_{samp}$</th>
<th>$u_\theta^{res}: min_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>25</td>
<td>0.45</td>
<td>35</td>
<td>0.25</td>
</tr>
<tr>
<td>15</td>
<td>35</td>
<td>0.15</td>
<td>25</td>
<td>0.25</td>
</tr>
<tr>
<td>75</td>
<td>35</td>
<td>0.35</td>
<td>35</td>
<td>0.15</td>
</tr>
<tr>
<td>135</td>
<td>35</td>
<td>0.35</td>
<td>35</td>
<td>0.25</td>
</tr>
<tr>
<td>195</td>
<td>35</td>
<td>0.25</td>
<td>35</td>
<td>0.15</td>
</tr>
<tr>
<td>270</td>
<td>35</td>
<td>0.35</td>
<td>35</td>
<td>0.15</td>
</tr>
</tbody>
</table>

Table 5.5: Comparison of the best DACE and empirical semi-analytical solutions for $u_r$

<table>
<thead>
<tr>
<th>$Re$</th>
<th>DACE: MSE</th>
<th>Empirical: MSE</th>
<th>DACE: $R^2$</th>
<th>Empirical: $R^2$</th>
<th>DACE: $n_{par}$</th>
<th>Empirical: $n_{par}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>8.5441e-15</td>
<td>1.5092e-14</td>
<td>1</td>
<td>0.99999</td>
<td>85</td>
<td>19</td>
</tr>
<tr>
<td>15</td>
<td>1.3274e-08</td>
<td>1.3188e-08</td>
<td>0.99984</td>
<td>0.99984</td>
<td>115</td>
<td>19</td>
</tr>
<tr>
<td>75</td>
<td>3.6484e-08</td>
<td>7.5786e-08</td>
<td>0.99998</td>
<td>0.99997</td>
<td>115</td>
<td>19</td>
</tr>
<tr>
<td>135</td>
<td>7.9056e-08</td>
<td>1.4699e-07</td>
<td>0.99999</td>
<td>0.99998</td>
<td>115</td>
<td>19</td>
</tr>
<tr>
<td>195</td>
<td>2.3474e-07</td>
<td>2.3454e-07</td>
<td>0.99999</td>
<td>0.99999</td>
<td>115</td>
<td>19</td>
</tr>
<tr>
<td>270</td>
<td>2.5016e-07</td>
<td>3.7837e-07</td>
<td>0.99999</td>
<td>0.99999</td>
<td>115</td>
<td>19</td>
</tr>
</tbody>
</table>

Table 5.6: Comparison of the best DACE and empirical semi-analytical solutions for $u_\theta$

<table>
<thead>
<tr>
<th>$Re$</th>
<th>DACE: MSE</th>
<th>Empirical: MSE</th>
<th>DACE: $R^2$</th>
<th>Empirical: $R^2$</th>
<th>DACE: $n_{par}$</th>
<th>Empirical: $n_{par}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>5.7812e-15</td>
<td>3.9045e-14</td>
<td>1</td>
<td>0.99999</td>
<td>115</td>
<td>11</td>
</tr>
<tr>
<td>15</td>
<td>1.0445e-08</td>
<td>1.2544e-07</td>
<td>0.99991</td>
<td>0.9989</td>
<td>85</td>
<td>11</td>
</tr>
<tr>
<td>75</td>
<td>1.6454e-07</td>
<td>5.7154e-07</td>
<td>0.99994</td>
<td>0.99981</td>
<td>115</td>
<td>11</td>
</tr>
<tr>
<td>135</td>
<td>7.9954e-07</td>
<td>8.7596e-07</td>
<td>0.99992</td>
<td>0.99991</td>
<td>115</td>
<td>11</td>
</tr>
<tr>
<td>195</td>
<td>1.2255e-06</td>
<td>1.1415e-06</td>
<td>0.99994</td>
<td>0.99996</td>
<td>115</td>
<td>11</td>
</tr>
<tr>
<td>270</td>
<td>1.8181e-06</td>
<td>1.4535e-06</td>
<td>0.99995</td>
<td>0.99996</td>
<td>115</td>
<td>11</td>
</tr>
</tbody>
</table>

The DACE modelling strategy produces accurate fits without making assumptions about the behaviour of the underlying data. However, it requires a large number of sampling points resulting in 85 to 115 overall number of parameters, compared to the empirical model only requiring 11 to 19 parameters. The flexibility of the model is an advantage since the same approach can be applied to other data to obtain reasonable approximations without modification to the model structure. This approach could therefore be useful when considering unsteady flow with vortex shedding.

The empirical models are based upon the identification of regions which follow identifiable functional forms. For the radial velocity, the splitting of the domain...
Figure 5.16: Comparison of the best performing DACE fits with the empirical model fits

with the second peak behind the sphere proved to be an effective strategy to isolate the wake feature which was fitted with a cross correlated exponential function. Since this feature was the greatest contributor to the overall error, the strategy produced good results. In the case of the angular velocity, the region
Chapter 5. *Semi-analytical bubble flow model investigation*

at the surface of the bubble was found to decay exponentially into the radial direction which also proved a good approximation. Based upon the accuracy of the fits and the number of parameters required, the empirical models present a suitable approximation for the use in the proposed bubble column simulation approach. The final residual (as depicted in Figure 5.17) shows that the significant functional forms have been captured when compared with Figure 5.4, and the remaining error is relatively small.

![Graphs showing residual comparison](image)

Figure 5.17: Final residual after Empirical model approximation for $Re = 135$

Since the objective of the bubble column modelling approach under development is the reduction of computational expense, the evaluation time of the two presented models is of interest. The averaged time to evaluate the solutions on a grid of 30158 points across the Reynolds range for both the radial and angular velocities is 0.0303 seconds for the empirical model and 0.9066 seconds for the DACE model. Although this is a significant difference, both these evaluation times can be considered negligible in comparison of the computation of similar fully converged CFD solution (using the Fluent CFD code [Fluent, 2006]) which has an average solution time of 138.7 minutes$^1$.

$^1$A desktop computer with an Intel i5 2.8 GHz processor and 4 GB of RAM was used for the computations.
5.4 Conclusion

It has been shown that the creeping and potential flow analytical solutions can account for significant portions of the flow field outside their idealized operating ranges with $Re \leq 270$. The non-linear deviations are captured through a statistical modelling strategy where a proposed empirical modelling strategy is compared with a DACE approach. For the DACE approach, an additional location dependent correlation function is introduced that weights the spatial correlation with respect to an optimizable region. This correlation function is shown to produce significantly lower MSE’s than the general powered exponential correlation function and mostly lower MSE’s than the previously proposed modified correlation function (in Chapter 4).

Both the empirical and DACE modelling approaches resulted in very accurate models of the spatial velocity flow fields, yielding $R^2$ values greater than 0.998 for all Reynolds numbers considered. The advantage of the DACE approach, is its flexibility to any type of data without any modification in the model structure. The proposed empirical modelling strategy requires the identification of regions following simple functional forms, which for the data considered produced accurate models for capturing the velocity residual with lower numbers of parameters compared to the DACE models. The results for the DACE model with the proposed correlation function is encouraging, considering that the model required very little analysis of the underlying data, whereas the empirical strategy relied on the careful identification of functional shapes. However, recognizing that each of the parameters of the spatial flow model will undergo correlation with respect to Reynolds number, based on the number of parameters, the empirical model seems to be the most suited for the purpose of the BCM. The cross correlation of the first stage parameters with respect to Reynolds number is investigated in the following chapter.
Chapter 5. *Semi-analytical bubble flow model investigation*
Chapter 6

Reynolds dependence of semi-analytical flow model

Given the developments presented in Chapter 5, an accurate model has been developed that approximates the flow field around a bubble at discrete Reynolds numbers. However, for the objective of developing a novel bubble column simulation approach (outlined in Chapter 3), the BCM is required as a continuous function of $Re$. Since the flow structures of the stage one BCM evolve smoothly with changes in Reynolds number, it is considered reasonable that the parameters of the stage one model could be described using functional forms. The present chapter examines the Reynolds dependence of the semi-analytical flow model to test whether this is true and what the corresponding functional forms might be. For this purpose the stage one BCM from Chapter 5 is considered in concise form in Section 6.1.1, followed by a sensitivity analysis of the error of the stage one model with respect to small changes in its parameters for both the empirical construction and the DACE approach (high order polynomial models are also considered) to establish the suitability of the given approaches for cross-correlation. The subsequent parameter responses with respect to $Re$ are analysed and fitted with appropriate models in Section 6.2.2, with the models cross validated in Section 6.2.3. The overall error is evaluated in Section 6.3 and conclusions drawn in Section 6.4.
6.1 The Bubble Cell Model stages of construction

The purpose of the BCM is to rapidly predict the velocity vector field around a bubble as a function of spatial position \(x\) and Reynolds number \(Re\). The overall construction of the BCM can be treated as a two stage fitting procedure as depicted in Figure 6.1. Here, the solution to the axisymmetric Navier-Stokes equations for the flow over a fixed sphere with a zero-shear-stress boundary condition [Magnaudet and Eames, 2000], is regarded as the “true velocity field”, \(u^t\). The stage one fitting process, which was the subject of the previous two chapters, involves approximating \(u^t\) for a series of Reynolds numbers within the operating range. The operating range has been selected as \(Re \leq 270\), which corresponds to the regime where air bubbles remain spherical in water [Clift et al., 1978]. The resulting velocity vector field is referred to as \(u^{m}\) while the stage one models are collectively termed \(f_{s1}\) with their parameters defined as \(\alpha\).

The first stage fitting process produces a set of \(\alpha’s\) for each \(Re\) considered. During stage two, the dependence of each of the \(\alpha’s\) with respect to \(Re\) is analysed and fitted with appropriate statistical models. The second stage models thereby approximate the behaviour of the first stage model parameters with respect to \(Re\) and are collectively defined as \(f_{s2}\) and its parameters as \(\gamma\). The final BCM can subsequently be evaluated as a combination of the stage one and stage two models that are functions of \(Re\), \(x\) and \(\gamma\). Accordingly, it would be possible to generate the entire velocity vector field in the vicinity of a bubble when given just the Reynolds number and the model.

6.1.1 Stage one model formulation

The linear combination of the creeping and potential flow analytical solutions, in the spherical coordinate system, has been found to serve as an useful first approximation model to \(u^t\), and can account for significant flow features with
few parameters [Coetzee et al., 2012b]. The equations from Chapter 5 (i.e., Eq. 5.10 to 5.11) are rewritten in terms of \( \alpha \) in Eq. 6.1 and 6.2. Here the superscript \( (\alpha^{1-19}) \) refers to the parameter number, whilst the subscript designates parameters for either the radial \( (\alpha_r) \) or angular \( (\alpha_\theta) \) velocity models.

\[
\begin{align*}
\mathbf{u}^{m,a}_r &= u_\infty \cos \theta \left( \alpha_r^{[1]} \left( 1 - \left( \frac{R}{r} \right)^3 \right) + \alpha_r^{[2]} \left( 1 - \frac{3}{4} \left( \frac{R}{r} \right)^{3} - \frac{1}{4} \left( \frac{R}{r} \right)^{3} \right) \right) \\
\mathbf{u}^{m,a}_\theta &= -u_\infty \sin \theta \left( \alpha_\theta^{[1]} \left( 1 + \frac{1}{2} \left( \frac{R}{r} \right)^3 \right) + \alpha_\theta^{[2]} \left( 1 - \frac{3}{8} \left( \frac{R}{r} \right) + \frac{1}{8} \left( \frac{R}{r} \right)^{3} \right) \right)
\end{align*}
\]  

(6.1)

(6.2)

Statistical models are required to account for deviations from the above mentioned analytical models. For this purpose, the domain is divided into two regions i.e., \( R_1 \) and \( R_2 \). For the purpose of the radial velocity, these regions are defined with respect to a critical angle \( \theta_c \), which is treated as a first stage parameter \( \alpha_r^{[17]} \) (see Figure 6.2).

The models that account for the residual in \( R_1 \) and \( R_2 \) respectively are given in Eq. 6.3 and 6.4. Collectively the first stage model for \( \mathbf{u}_r^{m} \) consists of 17 parameters.
Chapter 6. Reynolds dependence of semi-analytical flow model

Figure 6.2: Illustration of the critical angle \((\alpha_r^{[17]})\) that divides the domain into two regions, \(R_1\) and \(R_2\). The contours of the radial velocity residual (i.e., \(u_r^t - u_r^{m,a}\)) are also depicted.

\((\alpha_r^{[1-17]})\) and approximates the radial velocity across the Re operating range with \(R^2\) values ranging between 0.9968 - 0.9999. Two additional parameters i.e., \(\alpha_r^{[18,19]}\) are used as velocity and grid scaling parameters, where the grid scaling \((\alpha_r^{[19]})\) is constant with respect to Re.

\[
\begin{align*}
\left. u_r^{m,R1}\right|_{\theta=\alpha_r^{[17]}} &= -(\alpha_r^{[3]} e^{-\alpha_r^{[1]} r} + \alpha_r^{[5]} e^{-\alpha_r^{[9]} r} e^{-\frac{(-\theta - \pi)^2}{\alpha_r^{[7]} \alpha_r^{[9]} r + \alpha_r^{[9]}}}) + \alpha_r^{[10]} e^{-\alpha_r^{[11]} r^2} + \alpha_r^{[12]} e^{-\alpha_r^{[13]} r^2} + \alpha_r^{[14]} \\
\left. u_r^{m,R2}\right|_{\theta=\alpha_r^{[17]}} &= \left. u_r^{m,R1}\right|_{\theta=\alpha_r^{[17]}} e^{-(\alpha_r^{[15]} (\alpha_r^{[17]} - \theta)^2 + \alpha_r^{[16]} (\alpha_r^{[17]} - \theta))}
\end{align*}
\]

(6.3)

(6.4)

In the case of the angular velocity, \(R_1\) corresponds to the the bubble surface region (i.e., where \(r = R\)) and \(R_2\) the remainder of the domain. Subsequently the model \(u_r^{m,R1}\) (Eq. 6.5) approximates the residual at the bubble surface, while \(u_\theta^{m,R1}\) (Eq. 6.6) models the exponential decay into the radial direction. This strategy yielded accurate approximations of the data, with \(R^2\) ranging from 0.9974 - 0.9998 across the operating range. The model uses 9 parameters \((\alpha_\theta^{[1-9]}),\) with two
additional scaling parameters, $\alpha_{\theta}^{[10,11]}$, for velocity and grid scaling respectively (where $\alpha_{\theta}^{[11]} = \alpha_{r}^{[19]}$).

\[
\begin{align*}
\mathbf{u}_{\theta}^{m,R1} &= -\alpha_{\theta}^{[3]}(e^{-\alpha_{\theta}^{[4]}(\theta-\alpha_{\theta}^{[5]}\theta)^2} + \alpha_{\theta}^{[6]} \theta)erf(-\alpha_{\theta}^{[7]}(\theta - \alpha_{\theta}^{[5]})) \\
\mathbf{u}_{\theta}^{m,R2} &= \mathbf{u}_{\theta}^{m,R1} e^{-\alpha_{\theta}^{[9]}(r-R)+\alpha_{\theta}^{[9]}(r-R)\theta}
\end{align*}
\] (6.5)

6.2 Cross correlation

The $\alpha'$s are generated with respect to $Re$ by solving the axisymmetric Navier-Stokes equations at discrete Reynolds numbers with increments of 3 within the operating range, and fitting the resulting data with the stage one models introduced in the Section 6.1.1 (i.e., Eq. 6.1 to 6.6). To establish the suitability of the proposed stage one models for cross correlation, the sensitivity of the model error to the $\alpha'$s is investigated in Section 6.2.1. In Section 6.2.2 the responses of the $\alpha'$s are analysed and stage two models proposed. Finally each of the stage two models is cross validated to ensure that the estimators are not biased towards the training data set (Section 6.2.3).

6.2.1 Sensitivity of the stage one models

The propagation of error from the stage one models has the potential to severely influence the overall accuracy of the BCM. When the error of the stage one models is highly sensitive to small changes in $\alpha$, it places extreme accuracy requirements on the second stage estimators that could be infeasible. The sensitivity of the stage one model errors to changes in $\alpha$ is therefore an important consideration to establish the suitability of the given stage one models to cross correlation. In order to quantify the propagation of error, the gradient of the Mean Squared Error (MSE) to $\alpha_i$ is computed using the central difference approximation for each of the $i$ parameters (Eq. 6.7). To summarise the data produced, these gradients are averaged over all the model parameters (Eq. 6.8). The step size ($h$) is chosen as
\( h = 0.05 \alpha_i. \)

\[
\frac{dMSE_i}{d\alpha_i} \approx \frac{MSE_i(\alpha_i + h_i) - MSE_i(\alpha_i - h_i)}{2h_i} \quad (6.7)
\]

\[
\zeta = \frac{1}{n_{\text{par}}} \sum_{i=1}^{n_{\text{par}}} \frac{dMSE_i}{d\alpha_i} \quad (6.8)
\]

In addition to the first stage models presented in Section 6.1.1 (referred to as \textit{Emp} in this chapter), two other models i.e., \textit{Poly5} and \textit{DACE} are evaluated for comparison. The \textit{Poly5} model is based on the same strategy as the \textit{Emp} model, however 5\textsuperscript{th} order polynomial models are adopted for modelling the wake feature of \( u_r \) and the bubble surface residual of \( u_\theta \) (which offers similar accuracy than the exponential type models used for \textit{Emp}). The \textit{DACE} model corresponds to the model from Chapter 5. The final sensitivities are averaged over all the Reynolds numbers evaluated and reported in Table 6.1.

<table>
<thead>
<tr>
<th>Model</th>
<th>( \varsigma_{u_r} )</th>
<th>( \varsigma_{u_\theta} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textit{Emp}</td>
<td>( 8.3543 \cdot 10^{-7} )</td>
<td>( 2.2669 \cdot 10^{-5} )</td>
</tr>
<tr>
<td>\textit{Poly5}</td>
<td>0.0139</td>
<td>1.2733 \cdot 10^{-4}</td>
</tr>
<tr>
<td>\textit{DACE}</td>
<td>( 3.5320 \cdot 10^{-5} )</td>
<td>( 7.4431 \cdot 10^{-4} )</td>
</tr>
</tbody>
</table>

It is found that the \textit{Emp} model is significantly less sensitive to small changes in its parameters than the other two models. The \textit{Poly5} model is most sensitive to lack of fit due to multiplication of the errors with high order terms, which is especially evident for the \( u_r \) model. It is therefore found that even though high order polynomial models may be useful for fitting complex behaviour, the multiplication of model parameters with high order terms are poorly suited for cross correlation. The lower sensitivities of the proposed stage one models (\textit{Emp}), which follow from the use of exponential type functions, motivate their suitability for cross correlation. Since the ultimate performance of the second stage model depends directly on the stage one models, the sensitivities (\( \zeta \)) is a motivating factor behind the choice of the stage one sub-models.


6.2.2 Stage two models

To aid in achieving smooth responses of the first stage parameters with respect to \( Re \), each stage one fit was carried out using the parameter estimations from the previous fit as initial guesses, thereby warm starting the optimisation. For example, the parameter estimates for the \( Re = 270 \) surface is used as initial guesses for the \( Re = 267 \) surface, whose estimates are then used as initial guesses for the \( Re = 264 \) surface and so forth. The trust-region-reflective algorithm (described in Coleman and Li [1996]) is used to estimate the parameters for this purpose. This strategy proved effective since the changes in the velocity fields between consecutive \( Re \) (with the selected \( Re \) resolution of 3) is relatively small. The excellent initial guesses provided, following this strategy, resulted in smooth responses of \( \alpha \) with respect to \( Re \) where it was found that carrying out the procedure from high to low Reynolds numbers produced the most well behaved curves.

![Figure 6.3: Distinct parameters response \( \alpha_{r}^{[10]} \) (Eq. 6.9, \( R^2 = 0.9999 \)).](image)

From the responses observed for \( \alpha_r \) and \( \alpha_\theta \), 4 distinct families of shapes were
identified that can be used to classify these responses. To approximate these shapes, 4 models i.e., Eq. 6.9 to 6.12, are introduced that comprise of a combination of exponential and polynomial functions. The choice of these models is based on the combination of simple functions that yield very accurate fits. Such accuracy is required to limit the propagation of error from the second stage to the first stage models. Examples of the distinct shapes and the resulting second stage model fits are presented in Figure 6.3 to 6.6 which illustrate the accuracy of the proposed models.

\begin{align*}
  f_s^{[1]} &= \gamma_a \exp(-\gamma_b Re) + \gamma_c \exp(-\gamma_d Re) + \gamma_e \\
  f_s^{[2]} &= \gamma_a \exp(-\gamma_b Re) + \gamma_c \exp(-\gamma_d Re) + \gamma_e Re + \gamma_f \\
  f_s^{[3]} &= \gamma_a \exp(-\gamma_b Re) + \gamma_c Re^2 + \gamma_d Re + \gamma_e \\
  f_s^{[4]} &= \gamma_a Re + \gamma_b
\end{align*}
Chapter 6. *Reynolds dependence of semi-analytical flow model*

Figure 6.5: Distinct parameters response ($\alpha^{[9]}_9$, Eq. 6.11, $R^2 = 1.0000$).

### 6.2.3 Cross validation

Cross validation is a procedure that is performed to ensure generalizability of the models and to prevent overfitting of the data [Hawkins et al., 2003]. For this purpose Leave-One-Out Cross Validation (LOOCV), which has been shown to produce an almost unbiased estimator [Cawley and Talbot, 2004], is applied. The LOOCV entails removing a data point and fitting the model to the remaining points; the error is subsequently computed at the point that was removed. This process is repeated for all the data points such that the predictor at each point was fitted exclusive of the data at that point. The $R^2$ value for the cross validation data set is termed $q^2$. The subsequent results for both $\mathbf{u}_r$ and $\mathbf{u}_\theta$ including the stage two model, $R^2$, $q^2$ and second stage model parameters ($\gamma$) are summarised in Tables 6.2 and 6.3 respectively.
Chapter 6. Reynolds dependence of semi-analytical flow model

![Figure 6.6: Distinct parameters response ($\alpha_{[10]}^0$ Eq. 6.12, $R^2 = 1.0000$).](image)

Table 6.2: Summary of second stage models for $u_r$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model</th>
<th>$R^2$</th>
<th>$1 - R^2$</th>
<th>$\alpha^t$</th>
<th>$\gamma^t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{[1]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>0.9994</td>
<td>$5.9508 \cdot 10^{-4}$</td>
<td>0.9975</td>
<td>$-0.9923$, $0.1268$, $-0.3628$, $0.0196$, $0.9620$</td>
</tr>
<tr>
<td>$\alpha_{[2]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>0.9995</td>
<td>$4.7270 \cdot 10^{-4}$</td>
<td>0.9984</td>
<td>$1.1117$, $0.1190$, $0.4137$, $0.0189$, $0.0442$</td>
</tr>
<tr>
<td>$\alpha_{[3]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9991</td>
<td>$8.6387 \cdot 10^{-4}$</td>
<td>0.9979</td>
<td>$3.9429$, $-0.0013$, $-1.0488$, $0.1455$, $-0.0082$, $-2.6286$</td>
</tr>
<tr>
<td>$\alpha_{[4]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>0.9971</td>
<td>$2.8719 \cdot 10^{-3}$</td>
<td>0.9756</td>
<td>$0.0842$, $0.0048$, $-0.3402$, $0.1846$, $0.2285$</td>
</tr>
<tr>
<td>$\alpha_{[5]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>1.0000</td>
<td>$1.8120 \cdot 10^{-5}$</td>
<td>$1.0000$</td>
<td>$-227.7518$, $-0.0034$, $62.4114$, $0.0915$, $171.9904$</td>
</tr>
<tr>
<td>$\alpha_{[6]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.11)</td>
<td>0.9995</td>
<td>$4.9953 \cdot 10^{-4}$</td>
<td>0.9972</td>
<td>$-2.7510$, $0.1646$, $-2.1005 \cdot 10^{-5}$, $0.0188$, $6.1328$</td>
</tr>
<tr>
<td>$\alpha_{[7]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9996</td>
<td>$6.8362 \cdot 10^{-5}$</td>
<td>0.9996</td>
<td>$0.7998$, $0.0157$, $-1.6799$, $0.2946$, $-0.0012$, $1.6861$</td>
</tr>
<tr>
<td>$\alpha_{[8]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.11)</td>
<td>0.9991</td>
<td>$8.5175 \cdot 10^{-4}$</td>
<td>0.9981</td>
<td>$-0.6756$, $0.0632$, $-6.1544 \cdot 10^{-6}$, $0.0038$, $1.6115$</td>
</tr>
<tr>
<td>$\alpha_{[9]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9996</td>
<td>$4.4979 \cdot 10^{-4}$</td>
<td>0.9884</td>
<td>$0.1783$, $0.0414$, $0.6675$, $0.2729$, $-9.5692 \cdot 10^{-5}$, $0.0427$</td>
</tr>
<tr>
<td>$\alpha_{[10]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>0.9999</td>
<td>$1.1309 \cdot 10^{-4}$</td>
<td>0.9998</td>
<td>$-0.7514$, $-0.0045$, $1.9024$, $0.1199$, $-1.1393$</td>
</tr>
<tr>
<td>$\alpha_{[11]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.11)</td>
<td>0.9996</td>
<td>$3.6222 \cdot 10^{-4}$</td>
<td>0.9984</td>
<td>$-3.0895$, $0.1337$, $-3.3837 \cdot 10^{-6}$, $0.0141$, $5.0210$</td>
</tr>
<tr>
<td>$\alpha_{[12]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9990</td>
<td>$1.2111 \cdot 10^{-4}$</td>
<td>0.9980</td>
<td>$0.0820$, $0.0114$, $-0.2661$, $0.3426$, $-1.6542 \cdot 10^{-4}$, $0.1627$</td>
</tr>
<tr>
<td>$\alpha_{[13]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.11)</td>
<td>0.9996</td>
<td>$4.1084 \cdot 10^{-4}$</td>
<td>0.9992</td>
<td>$-0.2920$, $0.0476$, $-4.0164 \cdot 10^{-6}$, $0.0025$, $0.3989$</td>
</tr>
<tr>
<td>$\alpha_{[14]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.9)</td>
<td>0.9990</td>
<td>$1.0117 \cdot 10^{-3}$</td>
<td>0.7138</td>
<td>$0.1192$, $0.5549$, $0.0097$, $0.0066$, $0.0011$</td>
</tr>
<tr>
<td>$\alpha_{[15]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9982</td>
<td>$1.7620 \cdot 10^{-3}$</td>
<td>0.7249</td>
<td>$3.6415$, $0.0407$, $-3.7687$, $0.3547$, $-0.0014$, $1.4874$</td>
</tr>
<tr>
<td>$\alpha_{[16]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.11)</td>
<td>0.9966</td>
<td>$3.3976 \cdot 10^{-3}$</td>
<td>0.9955</td>
<td>$-0.4330$, $0.0339$, $-3.3157 \cdot 10^{-6}$, $0.0024$, $0.2042$</td>
</tr>
<tr>
<td>$\alpha_{[17]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.10)</td>
<td>0.9996</td>
<td>$3.5121 \cdot 10^{-4}$</td>
<td>0.9996</td>
<td>$-0.4997$, $0.0242$, $-0.0100$, $10$, $8.6518 \cdot 10^{-4}$, $1.9783$</td>
</tr>
<tr>
<td>$\alpha_{[18]}$</td>
<td>$f_{[4]}^2$ (Eq. 6.12)</td>
<td>1.0000</td>
<td>$4.7205 \cdot 10^{-5}$</td>
<td>0.9999</td>
<td>$6.1808 \cdot 10^{-4}$, $-0.0015$</td>
</tr>
<tr>
<td>$\alpha_{[19]}$</td>
<td>*</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>$7.6631 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>
Chapter 6. Reynolds dependence of semi-analytical flow model

Table 6.3: Summary of second stage models for $u_θ$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model</th>
<th>$R^2$</th>
<th>$1 - R^2$</th>
<th>$q^2$</th>
<th>$\gamma$'s</th>
</tr>
</thead>
<tbody>
<tr>
<td>$α_{[1]}$</td>
<td>$f_{[1]}$ (Eq. 6.9)</td>
<td>0.9995</td>
<td>5.2800 $\cdot 10^{-4}$</td>
<td>0.9981</td>
<td>$-0.8923, 0.1102, -0.4248, 0.0169, 0.9381$</td>
</tr>
<tr>
<td>$α_{[2]}$</td>
<td>$f_{[2]}$ (Eq. 6.9)</td>
<td>0.9996</td>
<td>4.1055 $\cdot 10^{-4}$</td>
<td>0.9988</td>
<td>$0.9849, 0.1031, 0.4793, 0.0163, 0.0714$</td>
</tr>
<tr>
<td>$α_{[3]}$</td>
<td>$f_{[3]}$ (Eq. 6.9)</td>
<td>0.9995</td>
<td>4.8107 $\cdot 10^{-4}$</td>
<td>0.9610</td>
<td>$1.6345, 0.0282, 6.7870, 0.2911, -8.1729 \cdot 10^{-4}, 0.6804$</td>
</tr>
<tr>
<td>$α_{[4]}$</td>
<td>$f_{[4]}$ (Eq. 6.9)</td>
<td>0.9991</td>
<td>8.7719 $\cdot 10^{-4}$</td>
<td>0.9991</td>
<td>$1.7435, -5.9937 \cdot 10^{-4}, -0.2816, 0.0224, -1.0249$</td>
</tr>
<tr>
<td>$α_{[5]}$</td>
<td>$f_{[5]}$ (Eq. 6.10)</td>
<td>0.9999</td>
<td>1.4909 $\cdot 10^{-4}$</td>
<td>0.9998</td>
<td>$0.0058, 0.0125, -0.0274, 0.1932, -1.7350 \cdot 10^{-6}, 3.1331$</td>
</tr>
<tr>
<td>$α_{[6]}$</td>
<td>$f_{[6]}$ (Eq. 6.9)</td>
<td>0.9987</td>
<td>1.2501 $\cdot 10^{-3}$</td>
<td>0.9987</td>
<td>$0.2508, -2.5290 \cdot 10^{-4}, -0.2605, 0.0241, -0.0139$</td>
</tr>
<tr>
<td>$α_{[7]}$</td>
<td>$f_{[7]}$ (Eq. 6.9)</td>
<td>0.9996</td>
<td>4.4667 $\cdot 10^{-4}$</td>
<td>0.9995</td>
<td>$-1.1482, 0.0093, -0.3961, 0.1128, 1.4839$</td>
</tr>
<tr>
<td>$α_{[8]}$</td>
<td>$f_{[8]}$ (Eq. 6.10)</td>
<td>1.0000</td>
<td>4.3419 $\cdot 10^{-5}$</td>
<td>0.9997</td>
<td>$0.137613, 0.0147, -11.9029, 0.1696, 0.0655, 24.4559$</td>
</tr>
<tr>
<td>$α_{[9]}$</td>
<td>$f_{[9]}$ (Eq. 6.10)</td>
<td>1.0000</td>
<td>4.5568 $\cdot 10^{-5}$</td>
<td>0.9997</td>
<td>$-4.3406, 0.0147, -3.7828, 0.1750, 0.0208, 7.8132$</td>
</tr>
<tr>
<td>$α_{[10]}$</td>
<td>$f_{[10]}$ (Eq. 6.12)</td>
<td>1.0000</td>
<td>5.6845 $\cdot 10^{-6}$</td>
<td>1.0000</td>
<td>$7.4614 \cdot 10^{-4}, -8.7633 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$α_{[11]}$</td>
<td>$f_{[12]}$ (Eq. 6.12)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$α_{[12]}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>7.6631 $\cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

The second stage models approximate the $α$’s accurately with all the responses being estimated with $R^2 > 0.997$. Through cross validation, the averaged $q^2$ for $α_r$ and $α_θ$ was determined as 0.9657 and 0.9954 respectively. Two outliers, i.e., $α_{[14]}$ and $α_{[15]}$, performed worse when the first data point (i.e., $Re = 3$) was removed, but overall it is concluded that the proposed second stage models provide good estimates irrespective of which data points are chosen to fit the model. The high accuracy of the second stage models show that the Reynolds dependent behaviour, in the range evaluated, is continuous with no noticeable discontinuous jumps observed.

6.3 BCM evaluation

With the stage two models constructed, the BCM can be evaluated as a function of $Re$ within the operating range (as depicted in Figure 6.1). Since the BCM approximates the axisymmetric Navier-Stokes equations for the appropriate flow scenario, the velocity field can be evaluated on a 3 dimensional grid. An example of the velocity vector field generated for $Re = 270$ is depicted in Figure 6.7.

The accuracy of the BCM is evaluated by comparing the velocity vector field generated by the BCM with a new validation data set obtained by the numerical solution of the Navier-Stokes equations at Reynolds numbers in between the Reynolds numbers of the training data set (i.e., $Re = 268.5, 265.5$, and so forth).
Figure 6.7: Scaled velocity vectors of the final BCM evaluated for $Re = 270$ (visualised with ParaView [Ahrens et al., 2005])
Chapter 6. Reynolds dependence of semi-analytical flow model

The $R^2$ statistic for both $u_r^m$ and $u_\theta^m$ are plotted against $Re$ in Figure 6.8, where the mean $R^2$ value for $u_r^m$ and $u_\theta^m$ is 0.9998 and 0.9987 respectively. It can therefore be concluded that the cross correlation performed has been successful, without significant loss in accuracy. This result is encouraging and shows that the cross correlation of the velocity vector field is possible, within the $Re$ range examined, given that suitable spatial models are used.

The average time consumed to evaluate the BCM within the Matlab environment [MATLAB, 2011] (averaged across the Reynolds numbers within the validation set) is 0.0395 seconds. Here the BCM is evaluated on the same grid as the validation data set (i.e., 31881 grid points) using a desktop computer\(^1\). The average time consumed to obtain fully converged numerical solutions ($\mathbf{u}^t$) was 138.7 minutes using the Fluent CFD code [Fluent, 2006]. The final model therefore satisfies the criteria stipulated in Chapter 3, i.e., an accurate model of the velocity vector field that can be rapidly evaluated, for application in the proposed bubble column simulator.

\(^1\)A desktop computer with an Intel i5 2.8 GHz processor and 4 GB of RAM was used for all computations.
Chapter 6. *Reynolds dependence of semi-analytical flow model*

Figure 6.8: $R^2$ statistic of cross correlated radial and angular velocity models ($u_r^M$ and $u_θ^M$) at different Reynolds numbers on validation data set

6.4 Conclusion

The stage one semi-analytical flow model from Chapter 5 describes the steady state velocity vector field around a bubble at discrete Reynolds numbers. To further the development the proposed bubble column simulation approach, this model is required as a continuous function of Reynolds number. For this purpose, the responses of the spatially dependent bubble flow model parameters ($α$) are analysed with respect to Reynolds number. The sensitivity of the model error to small changes in $α$ is quantified by central difference approximations and found to be relatively small compared to other potential models, thereby showing that small errors of the second stage models would not severely effect the accuracy of the cross correlated model.

The response of the parameters with respect to Reynolds number was found to follow well behaved curves, that could be classified into 4 distinctive families of curves. These distinctive shapes can be accurately approximated by way of 4
proposed algebraic models. Cross validation is applied, which shows no significant deviation in accuracy from the original fits. The comparison of the final model to a validation data set shows the cross correlated model to be accurate as well as quick to evaluate, thereby satisfying the criteria of the BCM. The principle barrier towards the application of the BCM simulation approach has therefore been overcome through the development of the two stage BCM. The coupling of the BCM within a macro reactor framework is investigated in the following chapter.
Chapter 6. *Reynolds dependence of semi-analytical flow model*
Part III

Model application & Conclusions
Chapter 7

Application of the Bubble Cell Model

With the BCM development concluded in Chapter 6, the application of this model toward the prediction of whole-column simulations can be investigated. For this purpose, the centre of mass of each bubble is tracked within a Lagrangian framework, while the liquid phase is considered within an Eulerian reference frame. The coupling between the two phases is achieved by imposing the regions surrounding the centre of mass of individual bubbles with velocity fields predicted by the BCM for the appropriate Reynolds numbers. The domain outside of the BCM regions is resolved by numerically solving the Navier-Stokes equations. To this end, a series of methods are introduced in this Chapter that serve to address the technical challenges posed by coupling the BCM regions with the surrounding fluid that is solved numerically with CFD procedures.

To demonstrate the principle of the BCM based simulator the case of a single bubble rising and two bubbles rising are compared with similar Volume-Of-Fluid (VOF) simulations. The simulation of full-scale bubble columns is beyond the scope of the present study and these cases are selected to illustrate the development of the flow pattern in the surrounding fluid and the two-way coupling that can be achieved with the BCM approach together with the computational demand.
Chapter 7. Application of the Bubble Cell Model

The solution procedure is outlined in Section 7.1 with the generation of the velocity fields using the BCM treated in Section 7.2. The imposition of the BCM velocity field onto the Eulerian grid is examined in Section 7.3 followed by the BCM tracking in Section 7.4. Two case studies are evaluated in Section 7.5 comparing the VOF and BCM approaches. Conclusions are drawn in Section 7.6.

### 7.1 Solution procedure

One method of applying the BCM for the simulation of gas-liquid flow follows from imposing the flow fields around individual bubbles with the velocities predicted using the BCM (this concept is illustrated in Figure 7.1). To achieve this objective, the fluid flow outside of the BCM regions needs to be resolved, which can be accomplished through the application of an unsteady incompressible CFD solver. Such a CFD solver must be adapted to allow for the coupling of the Euler and Lagrange frameworks, where the element of the Lagrange framework viz. the BCM, is a new model. Since commercial packages do not offer this degree of flexibility, significant technical development is accepted to achieve this objective. The OpenFoam CFD libraries [Weller et al., 1998] is subsequently employed, due to the inherent flexibility Opensource code offers to explicitly implement and modify routines.

The solution procedure follows from the introduction of additional steps in the general pressure velocity coupling scheme (see Figure 7.2). Here the centre of mass of each bubble is tracked (track bubble centre of mass), followed by the identification of the cells in the regions surrounding the bubble centre of mass (obtain BCM region cells). The relative velocity vector of each bubble from the Lagrangian framework (represented in Figure 7.1 as $u_{rel}$) is used to determine the direction and Reynolds number for the flow over each bubble, which, together with the spatial location of the BCM region cells, is used to evaluate the BCM (evaluate BCM). The subsequent BCM velocities is then imposed on the Eulerian grid (impose BCM velocities). The discretised momentum equations are then solved (solve momentum predictor), followed by the pressure-velocity
Chapter 7. Application of the Bubble Cell Model

Figure 7.1: The Bubble Cell Model (BCM) concept, the subject of this study.

coupling loop, where the hydrostatic pressure is imposed in the BCM regions (impose hydrostatic pressure) and the Poisson Pressure Equation is solved (solve Poisson Pressure Equation). The application of these techniques is discussed in the following sections.

Another method of coupling the BCM to the outside fluid regions follows from the adding the BCM regions as a momentum sources rather than imposing the velocity field. This “additive” approach falls outside the scope of the current model application, however, it should be noted that there is potential in coupling the BCM following different techniques.
Chapter 7. Application of the Bubble Cell Model

7.2 Evaluating the BCM

To evaluate the BCM with respect to spatial position, the location of the cells falling within the BCM regions is required. A brute force approach would be to loop over all the cells in the grid and evaluate whether they fall within these regions. However, since the selection of these cells needs to be carried out for each bubble at every time step it would increase the computational expense of the solver, which is what the BCM approach is aiming to avoid. Therefore it is proposed to exploit the relation between cells of a structured orthogonal grid to identify these cells in an efficient manner.

The numbering of the cells for the orthogonal mesh occurs in an incremental manner. The convention adopted is cell numbering by increments of 1 in the \( x \) direction. Therefore, by knowing the cell address of the centre of mass of a bubble, the addresses of the surrounding cells can be obtained from the series of incremental numbers for the cells in each \( x \) direction row. The procedure for selecting the cells and evaluating the BCM is outlined in Figure 7.3 and discussed below.
Chapter 7. Application of the Bubble Cell Model

The following procedure is carried out for all the bubbles being tracked at each time step. To initialize the vector containing the cell addresses, the number of cells is estimated by dividing the volume of a sphere (for the 3 dimensional case) or the area of a circle (for the 2 dimensional case) by the volume or area of each cell. The cell addresses of the region contained in an enclosed spherical region around the bubble centre of mass is obtained as the series of numbers from the first to the last cell in each $x$-direction row within this region, where the number of cells in each row is calculated as the local $x$-component of the sphere divided by the $x$-cell-length. The BCM domain is based on the regions where the highest gradients occur. Since the velocity gradients occur in a smaller region at the frontal region of the bubble compared to the rear, where the bubble wake is present, this domain can better be approximated by the region enclosed by two ellipsoids (see Figure 7.4). Therefore, from the cells selected in the spherical domain, some of the cells are not contributing information and therefore should be removed from the BCM domain. The equations for the top and bottom ellipsoids are given by Eq. 7.1 and 7.2 respectively, where the coefficients are chosen as $\delta_{xz} = 1.25$, $\delta_y = 2$ and $\delta_R = 5$, that give rise to a smaller frontal region compared with the rear (these coefficients may selected as optimisation parameters in further study).
Chapter 7. Application of the Bubble Cell Model

\[
\sqrt{(\delta_{xz}x)^2 + (\delta_yy)^2 + (\delta_{xz}z)^2} < \delta_R R 
\]  \hspace{1cm} (7.1)

\[
\sqrt{(\delta_{xz}x)^2 + (y)^2 + (\delta_{xz}z)^2} < \delta_R R 
\]  \hspace{1cm} (7.2)

Figure 7.4: The volume enclosed by the 2-ellipsoidal domain is shown in blue with the volume of the spherical bubble represented by the meshed spherical region.

Since the 2-ellipsoidal region is aligned with the bubble wake, it is directional (in contrast with a spherical region). The domain is therefore rotated with respect to the bubble velocity vector by multiplication with rotation matrices \( M_x \) and \( M_z \) (Eq. 7.3 and 7.4). Here \( \theta_{a,x} \) and \( \theta_{a,z} \) represent the angles that the bubble velocity vector make with the \( x \) and \( z \) axes respectively. The cells enclosed within the 2-ellipsoidal region are identified by looping over the cells in the spherical region and testing whether they fall within this rotated 2-ellipsoidal domain. This procedure
Chapter 7. Application of the Bubble Cell Model

of first selecting a spherical region and then testing which of the cells fall within the rotated 2-ellipsoidal domain is advantageous to looping over all the cells in the domain\(^1\).

\[
M_x = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \theta_{a,x} & -\sin \theta_{a,x} \\
0 & \sin \theta_{a,x} & \cos \theta_{a,x}
\end{bmatrix}
\]

(7.3)

\[
M_z = \begin{bmatrix}
\cos \theta_{a,z} & -\sin \theta_{a,z} & 0 \\
\sin \theta_{a,z} & \cos \theta_{a,z} & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

(7.4)

With the ability to rotate the BCM regions, the approach can be applied to situations where the bubble motion occurs in more than one direction, which is often the case (e.g., Section 2.3.3). The function written for selecting the cells (\texttt{cellsOccupied}) as discussed above is written in C++ using OpenFoam data types and is included in Appendix C.

With the appropriate cells identified, the BCM velocity vector field can be evaluated. Since the BCM was constructed in spherical coordinates, the grid points of the selected cells are converted from Cartesian to spherical coordinates. The second stage models introduced in Chapter 6 (which are functions of Reynolds number) are first evaluated (Eq. 6.9 to 6.12). These responses are subsequently used to evaluate the stage one models introduced in Chapter 5, which are functions of spatial position (Eq. 6.1 to 6.6). The resulting velocity vector field is then converted from spherical to Cartesian velocity vectors, since the macro flow

\(^1\)A comparative test was conducted in MATLAB [2011] where 7697 BCM cells were selected from a domain of 75 \times 200 \times 75 cells. By using the orthogonal relation, it took 0.0705 seconds to select the appropriate cells compared with 0.3502 seconds expended when looping over all the cells and testing whether they fall within the region. This result shows the advantage of the proposed cell selection method, however, relative to the overall computation time these values are still small and subsequently does not preclude the use of unstructured grids.
Chapter 7. Application of the Bubble Cell Model

simulation is in the Cartesian coordinate system. The function for evaluating the BCM (getBCMVelocities) is included in Appendix C.

7.3 Imposing the velocity vector field

With the BCM velocities and the corresponding cells known, the next step (see Figure 7.2) is to impose the predicted velocity vector field in the relevant cells. It is important that these solutions do not contribute to the overall error of the system, such that the BCM velocities are modified by the solver (i.e., the velocities predicted by the BCM should not be “solved” together with the velocities of the rest of the domain). One way of imposing the velocity in a given cell, is by modification of the algebraic system of equations (the system of algebraic equations is introduced in Section 2.5.1.6 of the literature review) to remove the influence of the cells concerned from the linear system solver. The procedure to achieve this is outlined below.

Consider the discretised linear algebraic equation for an individual cell, given in Eq. 2.31 and repeated below.

\[ a_P \phi_P + \sum_N a_N \phi_N = R_P \]  

To impose a given value \( v \) for \( \phi \) in the present cell (i.e., \( \phi_P = v \)), set the source term \( R_p \) equal to the product of \( v \) and the matrix coefficient for the present cell \( a_P \) while specifying the contribution of the neighbouring coefficients \( a_N \) as zero (see Eq. 7.5 to 7.7).

\[ \phi_P = v \]  
\[ R_p = va_P \]  
\[ a_N = 0 \]
This modification of Eq. 2.31, results in the trivial solution for $\phi_P$ as shown in Eq. 7.8.

$$a_P \phi_P + \sum_{N} (0) \phi_N = a_P v$$

Through the procedure described above it is possible to set the solution of a given cell to a specified value with the inclusion of the influence to the neighbouring cells. This can be achieved using the `fvMatrix::setValues` routine in the OpenFoam libraries.

### 7.4 Tracking the BCM centre of mass

The centre of mass of individual bubbles is solved in a Lagrangian reference frame using a force balance of the buoyancy and drag forces. The drag coefficient is computed based on the terminal velocity of a bubble (see Eq. 2.18). This force balance is solved using the 4th order Runge-Kutta method [Dormand and Prince, 1980]. To account for possible gradients in the approaching velocity e.g., a shear velocity profile, the velocity distribution in the cells just ahead of the BCM is considered. These cells are termed the free stream cells and defined as the frontal cells of the spherical BCM region that are not enclosed by the top ellipsoid. The number of the free stream cells is denoted as $n_{fscells}$.

The free stream velocity vector ($u_{fs}$) is defined here as the average velocity on the Eulerian grid over the free-stream cells (Eq. 7.9). The rotation of $u_{fs}$ is determined from the local spatial distribution of the velocities in the free stream cells, whereby the local coordinate (centred around the BCM) is multiplied with the velocity, such that a bias of velocity towards a particular region will correspond with an appropriate rotation ($\theta_{mx}$ and $\theta_{mz}$). In this way, the BCM can respond to a shearing free stream velocity profile. The factors $\kappa_{fs}$, $\kappa_{x}$ and $\kappa_{z}$ are used to weight the response of the BCM towards free-stream velocity fields, such that accurate two-way coupling may be achieved.
7.5 BCM based simulator case study

The application of the BCM is evaluated for two test cases i.e., a single bubble rising and two bubbles rising. The single bubble case serves to demonstrate the realistic bubble wake and flow pattern development throughout the entire domain while the two bubble case demonstrates the two-way coupling that can be achieved, whereby the influence of the bubbles on the medium and in turn the influence of the medium on the bubbles is predicted. The results from the BCM simulations are compared with similar Direct Numerical Simulation (DNS) simulations. This comparison is done since the DNS simulations represent the most fundamental treatment of multiphase flow and the quantitative bubble scale flow information produced is not available experimentally. Subsequently, the test cases are designed for this study to evaluate the capabilities of the BCM based simulator to predict the bubble induced flow phenomenon at a reduced computational expense to equivalent DNS simulations. The type of DNS approach employed is the Volume-Of-Fluid (VOF) method following the implementation suggested by Ubbink [1997] and Rusche [2002].

Due to the computational expense (CPU time and memory requirement) of the VOF approach, simulations are performed in 2D. It should be noted that the BCM approach is capable of 3D simulations, since the BCM is based on the

\[
\mathbf{u_{fs}} = \frac{\kappa_{fs}}{n_{fscells}} \sum_{celli=0}^{n_{fscells}} \mathbf{u}[celli]\]  
(7.9)

\[
m_x = \sum_{0}^{n_{fscells}} x_c u_y[celli]\]  
(7.10)

\[
m_z = \sum_{0}^{n_{fscells}} z_c u_y[celli]\]  
(7.11)

\[
\theta_{mx} = \tan^{-1}(\kappa_x m_x)\]  
(7.12)

\[
\theta_{mz} = \tan^{-1}(\kappa_z m_z)\]  
(7.13)
axisymmetric flow field around a bubble. The same orthogonal mesh is used for all simulations which consists of 208250 cells. The velocity boundary conditions on the walls are free-slip, while a zero-gradient Neumann condition is applied at the outlet at the top of the domain. The dimensions of the domain is specified as $15d$ by $25d$, where $d$ represents the diameter of the bubble being simulated ($d = 1\text{mm}$).

7.5.1 Single bubble rising

The single bubble test case consists of a $1\text{ mm}$ diameter air bubble rising in initially stagnant water. The terminal velocity used to compute the drag coefficient is determined from Figure 7.5. The simulation time selected is $0.1\text{s}$ with write intervals of $0.0015\text{s}$. The time step is adjusted such that the maximum CFL number\footnote{The CFL condition is an acronym for Courant-Friedrichs-Lewy that was first described in 1928 and remains a popular measure to select appropriate time step sizes.} [Bakhvalov, 2001] remains below $0.5$ (see Eq. 7.14, where $u$ is the velocity, $\Delta t$ the time step and $\Delta x$ the cell length). Typically a $CFL < 1$ is required to avoid numerical instability [Bakhvalov, 2001].

$$CFL = \frac{u\Delta t}{\Delta x}$$ (7.14)

The rise velocities for both the VOF and BCM simulations are plotted in Figure 7.6. For the VOF case, the rise velocities are calculated by determining the centre of mass of the bubble at each time step. The rise velocities correspond to what is expected from experimental results published by Clift et al. [1978] (depicted in Figure 7.5), however, since there is no absolute benchmark and the behaviour is similar, both responses are considered of similar accuracy. The velocity vector fields for both these simulators are presented at $t = 0.0375$, $0.075$ and $0.0975$ seconds in Figure 7.7 and 7.8 respectively. In addition, for a qualitative comparison the experimental rise velocity of a $1.58\text{ mm}$ bubble is shown in Figure 7.9.

From the results presented, it can be seen that the BCM approach simulates
Chapter 7. Application of the Bubble Cell Model

Figure 7.5: Rise velocities of air bubbles in both clean and contaminated water (at 20°) for different bubble sizes. The top curve represents the terminal velocity for a clean bubble while the bottom curve corresponds to a contaminated system. The test cases are marked i.e., a clean bubble of 1 mm and 0.9 mm diameter which correspond to terminal velocities of approximately 19 m/s and 18 m/s respectively (from Clift et al. [1978]).

the development of a realistic wake, as well as the ensuing flow pattern within the column outside of the BCM regions. The flow patterns between the two approaches are very similar, with minor discrepancies. A slight deviation in the rectilinear bubble path of the VOF simulation can be seen in Figure 7.8c, however, this may be considered due to numerical instability rather than a physical feature. Furthermore, the general shape of the wake corresponds with the experimental observations by de Vries [2001]. The major advantage that the BCM approach offers is that the high gradient regions around the bubble is predicted using a semi-analytical model that can be rapidly evaluated. The results show that the application of this model in the BCM regions results in the realistic development of the flow pattern throughout the domain. The comparison in run time of the
two models on the same computer\(^1\) for 0.1 seconds of simulation time was 1.97 hours for the VOF simulation compared with 16 minutes for the BCM approach.

![Figure 7.6: A comparison between the rise velocities using the VOF method and the BCM approach for a single bubble test case. The average percentage difference between the velocities is 5.22\%.](image)

### 7.5.2 Two bubbles rising

The results from the two bubbles rising case demonstrate the two-way coupling that can be achieved with the BCM approach. In this case, two bubbles of 1 \textit{mm} and 0.9 \textit{mm} respectively is simulated. The smaller bubble is initialized at a slightly higher position in the column with respect to the larger bubble such that the 1 \textit{mm} bubble rises in the wake of the 0.9 \textit{mm} bubble. The resulting rise velocities is presented in Figure 7.10. Comparing the rise velocities from the two bubble case with that of the single bubble test case, it is evident that the 1 \textit{mm} bubble (which rises in the wake of the smaller bubble) exhibits an increased velocity of approximately 5\%. This increase in the 1 \textit{mm} bubble velocity

---

\(^1\)The computer used to run the simulations is a Intel i7 Q740 laptop with 3.8 Gb of RAM running on the Ubuntu Linux operating system
is observed for both the BCM and VOF cases and is similar. The trajectories of the two approaches are compared in Figure 7.11. The paths exhibit comparable deviation of the 1 mm bubbles from a rectilinear path. This deviation together with the increase in velocity of the 1 mm bubble, demonstrates how the wake of the first bubble influences the trajectory of the second bubble with comparable results between the two simulators.
Figure 7.8: Velocity vector fields for the VOF single bubble test case at three different time steps.

The ensuing velocity vector fields throughout the domain are compared in Figure 7.12 and 7.13. As in the previous case it is shown that although the fields are not exactly the same, the flow patterns are similar and the velocity magnitudes are of the same order. Furthermore, it is seen with the BCM approach, even as the two bubbles move close together, the flow pattern remains realistic and comparable with that of the VOF approach. Subsequently, the major features of the flow
Section 7. Application of the Bubble Cell Model

Figure 4.1: The single-threaded wake behind a rectilinear rising bubble ($r_{eq} = 0.79 \text{ mm}$). On the left the XZ view and on the right the YZ view. The black areas are part of the reference system outside the water tank. The walls of the tank and the mirror inside the tank are over 20 bubble radii away from the bubble.

These points are 0.5 cm. It can be seen in Figure 4.1 that the reference points between the two perpendicular views are displaced vertically, which indicates that both views are not perfectly aligned. This misalignment is compensated for in the analysis. The reference system is placed outside the water tank and therefore will not influence the motion of the bubble. The walls of the water tank and the mirror placed inside the tank are over 50 bubble radii away from the bubble. As a consequence the motion is not influenced by wall effects.

Although it is not (clearly) visible in the images, there exists a vertical temperature gradient in the water column. The bubble drags some colder water in its wake. For reference purposes, denote the direction from left to right in both projections as positive. In a horizontal plane the temperature changes with position in both projections: i.e., from left to right, in the plane outside the wake warm, inside the wake colder and outside the wake again warmer. A negative temperature gradient in horizontal direction, or in other words a positive gradient in refractive index, is visualised with a positive gradient in the intensity (a lighter area). A positive gradient in the temperature results in a darker area. As a consequence the single-threaded wake is visible as a lighter and a darker streak. The relation between grey scale and temperature gradient is connected to the orientation of the schlieren gradient filter. The schlieren images clearly show the stable single-threaded wake.

Figure 7.9: The experimentally observed wake behind a rectilinear rising air bubble of $1.58 \text{ mm}$ diameter in water. On the left the XZ view and on the right the YZ view. (From de Vries [2001]).

Patters between the two approaches are similar, however minor discrepancies exist. These differences could potentially be attributed to the coupling method i.e., the imposition of the BCM vector field, rather than an additive influence through a momentum contribution. This present work emphasises the BCM development and therefore the investigation of different coupling strategies is outside the scope of the present work, however, this identifies an area for future investigation.

The computational times required to produce these solutions were 2.85 hours for the VOF simulation compared with 12.8 minutes for the BCM approach that represents a substantial saving in computation times. These results together with the single bubble computational demands are tabulated in Table 7.1. The significant reduction in computational expense coupled with the comparative bubble scale flow fields of the BCM based simulation, satisfies the objectives of this study set out in Chapter 3.

It is interesting to note that the computation time of the BCM based simulator decreased when simulating two bubbles compared with the single bubble case,
Chapter 7. Application of the Bubble Cell Model

Figure 7.10: A comparison between the rise velocities using the Volume-Of-Fluid method and the BCM approach for the two bubble test case. The average percentage difference between the velocities for the 1 mm bubble is 4.59% and 7.40% for the 0.9 mm bubble.

while comparatively the computation time increased for the VOF approach. This could be explained by the CFD solver effectively solving fewer cells in the BCM case (since more cells are predicted using the BCM) while the VOF solver has the same amount of cells but with higher gradients. This reduction in computational load with the addition of an extra bubble could have positive implications when many bubbles are simulated with the BCM approach, however, such cases will require a larger grid that will trade-off the computational cost.

Table 7.1: Computational performance of VOF and BCM approaches for 0.1 seconds of simulation time.

<table>
<thead>
<tr>
<th>Case</th>
<th>VOF</th>
<th>BCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single bubble</td>
<td>7075 s</td>
<td>962 s</td>
</tr>
<tr>
<td>Two bubbles</td>
<td>10246 s</td>
<td>766 s</td>
</tr>
</tbody>
</table>
Figure 7.11: Bubble trajectories for the two bubble case computed with the VOF and BCM simulators.
Chapter 7. Application of the Bubble Cell Model

Figure 7.12: Velocity vector fields for the BCM two bubble test case at three different time steps.
Figure 7.13: Velocity vector fields for the VOF two bubble test case at three different time steps.
Chapter 7. Application of the Bubble Cell Model

7.6 Conclusion

A unique gas-liquid simulation approach has been proposed and investigated. This approach relies on the Bubble Cell Model developed in the previous chapters and the coupling with an unsteady Navier-Stokes solver. The cases of a single bubble rising and two bubbles rising were investigated where it is shown that the BCM approach is capable of predicting bubble scale flow information at significantly reduced computational expense compared with the Volume-Of-Fluid technique. This serves to prove the concept of the proposed methodology, where the use of a semi-analytical model in the high gradient regions around individual bubbles can significantly reduce computational demand.

It should be noted that there was significant computational effort in the construction of the BCM, which is currently only valid for spherical bubbles in the range of $Re \leq 270$. However, the use of this model in the proposed bubble simulations mean that these solutions are stored as statistical models which can be rapidly evaluated, thereby reducing the computational demand of future simulations. The BCM approach is shown to successfully simulate bubble induced flow patterns for two relatively simple cases, which invites the extension of the semi-analytical model to non-spherical bubbles and higher Reynolds numbers. Furthermore, there is potential to increase the accuracy of the model by investigating different coupling strategies such as an additive momentum approach instead of imposing the BCM velocity field. There is also significant scope to extend the BCM to predict concentration and temperature profiles to predict mass and heat transfer as well as the potential application of the BCM within a Population Balance Modelling (PBM) framework.
Chapter 7. Application of the Bubble Cell Model
Chapter 8

Conclusions

The focus of this study is the reduction of the computational expense associated with simulating gas-liquid flow occurring in bubble columns by accounting for the micro-flow fields around individual bubbles with a surrogate model that can be rapidly evaluated.

“By treating the micro-flow field around a bubble as the fundamental building block of the bubble column simulation and modelling this element with statistical models, dependent on spatial position and Reynolds number, a significant amount of computational expense can be avoided.”

The testing of this hypothesis required the development of such a surrogate model, which is not trivial due to the non-linear nature of these flow fields. For this purpose, a two stage fitting procedure is utilised, where stage one entailed approximating the spatial flow field at discrete Reynolds numbers, while the second stage involved describing the Reynolds number dependence of the stage one model parameters. During the construction of the stage one model, different strategies were evaluated, where it was found that a combination of the creeping and potential flow analytical solutions can account for important flow features. The remainder consisted mainly of the non-linear wake, which was approximated through statistical models.
For the second stage model, it was hypothesised that since the flow features develop gradually with respect to Reynolds number, the model parameters of the stage one model would exhibit similar smooth responses with small increments in Reynolds number. This was found to be correct, which allowed the first stage parameter responses to be described by the second stage models. The completion of the BCM allowed the velocity vector field around a bubble to be rapidly evaluated for a given Reynolds number within the operating range.

The application of the BCM within a macro reactor framework was evaluated by imposing the velocities generated by the BCM around the centre of mass of individual bubbles in a Euler-Lagrangian framework. This was achieved by the modification of the linear system of equations; such that the BCM velocities do not contribute to the overall error of the CFD simulation. The velocity vector fields of the BCM are rotated to align with the relative velocity vector of the bubble using rotation matrices. The simulation was evaluated for a single bubble and two bubbles rising and compared to similar cases using the Volume-Of-Fluid (VOF) method using an established simulator and methodology. Here it is found that the BCM approach produces similar results compared to the VOF method, however, at significantly reduced computational expense which is approximately an order of magnitude faster. This simple case study proves the basic hypothesis, whereby significant reduction in computational expense is observed following the BCM approach. The discount in computational expense increases the feasibility of model-based optimisation while the BCM provides high levels of flow information at the bubble scale.

The positive result from this study invites additional work that stems naturally from what has been presented. The extension of the BCM operating range will widen the applicability of this approach to more industrial relevant problems. Direction on how these issues may be dealt with is discussed below.
8.1 Future direction

Beyond $Re \leq 270$

There are two main issues when going beyond $Re \leq 270$ i.e., non-spherical bubble shapes and transient bubble wakes. The non-spherical bubbles could be predicted through empirically correlated aspect ratio models (as presented by Loth [2008]). These models are dependant on the Weber (factors in the surface tension, subsequently the Eötvös number could also be used) and Reynolds number. For the consideration of non-spherical bubbles, the BCM should be constructed as a function of both Reynolds and Weber (or Eötvös number). The change in Weber number will be accompanied by a change in aspect ratio which can be predicted by empirical models (this will also have to be considered when generating the CFD solutions used to fit the BCM). One method of modifying the BCM for the non-spherical case would be to transform the current solution using a scale transformation matrix to fit the spherical boundary onto an ellipsoid, scaling the velocity vector field accordingly. Some error can be expected with this process and this will have to be quantified to see how much additional modelling is required. If the error is significant, it might be better to reconstruct the BCM for each of the different aspect ratio’s using the form of the BCM proposed in this study as a starting point.

For the transient bubble wakes, an additional point at each Reynolds number could be considered, where the wake reaches its maximum amplitude. Subsequently, it would be possible to model the transient wake by assuming symmetry and using two points (i.e. wake at zero deviation and extreme amplitude) and interpolating between them based on the oscillation frequency of the wake (which could be found from the CFD simulations).

The fitting of the residual with the DACE model will follow exactly the same procedure as described in Chapter 5, since the method does not depend on the form of the data. It has been shown in this study that the DACE model is capable of accurately approximating non-linear flow structures and it can reasonably be expected that this will not require significant change when considering changes
in the flow structures. The empirical modelling strategy on the other hand will require analysis of the flow structure to examine whether the models proposed in this study remain applicable and what modification will be required. This shows the advantage of the DACE approach and why it is considered a favourable strategy when going beyond $Re \leq 270$, since in principle it can approximate complicated flow structures without detailed analysis of the underlying features.

**Bubble break-up and coalescence**

Bubble break-up and coalescence is an important phenomenon that should be considered when modelling the heterogeneous flow regime since this effect directly influences the mass and heat transfer characteristics. The coalescence of bubbles could be modelled with the BCM approach by checking the proximity of the bubbles to one another and if two bubbles are sufficiently close and on a collision trajectory, to collapse the two BCM’s into one with the appropriate Reynolds number. In addition to collision detection, a collision efficiency parameter may also be used (as presented by van den Hengel et al. [2005]) to account for the effects of surface tension and the time to drain the film between two bubbles.

Bubble break-up can occur when a turbulent eddy collides with a bubble. The probability that a bubble will break after it collision with a turbulent eddy can be determined by the often cited break-up model of Luo and Svendsen [1996]. The break-up efficiency, in a similar manner to the coalescence efficiency, can be employed based on the collision of bubbles with eddies.

**Wall effects**

It its current state, wall effects are not included in the Bubble Cell Model. For the two test cases (in Chapter 7), the size of the domain was chosen to have a negligible effect on the behaviour of the bubbles and the walls modelled as free-slip boundary conditions. Furthermore, it has been discussed by Clift et al. [1978] and confirmed with simulation by Krishna et al. [1999] that bubble rise velocity is independent of wall effects when the ratio of the bubble diameter to column
 CHAPTER 7. APPLICATION OF THE BUBBLE CELL MODEL

Diameter is less than 0.125, where this ratio is 0.067 in the cases simulated. However, this is remains an important effect to be considered when modelling bubble columns. Wall effects can be accounted for by a force coefficient that is dependent on the distance of the bubble to the wall (e.g., the ratio of the bubble size to the distance of the bubble center to the wall). Several such coefficients are reported in literature [Fukagata et al., 1999; Brenner, 2005] and could be applied within the current BCM simulator framework. This relatively simple method would have to be evaluated before application to problems. Another method would be to make the treatment of near wall flow part of the BCM construction such that the distance to a wall is considered as an additional parameter for the prediction of the flow field. However, the introduction of an additional variable to the BCM will significantly increase the construction effort of this model. In such a case, the use of the DACE strategy may become more advantageous due to its flexibility to different flow structures.

**Heat and mass transfer**

The inclusion of statistical mass and heat transfer models has the potential to further increase the usefulness of the approach. Both of these phenomena can be characterised by dimensionless numbers (e.g., the Prandlt number and the Schmidt number) and since they are based on the same form of governing equations, heat and mass transfer analogies exist that could simplify computation. Therefore, a similar approach to what has been proposed in this text can be applied to predict heat and mass transfer in conjunction to momentum transfer to extend the usefulness of the proposed approach.

**8.2 Closure**

The approach presented in this thesis represents a fundamentally different way of approximating the flow around bubbles and is shown to be effective for simple cases. A framework for both the construction of the surrogate micro-flow field
model (using a two stage fitting process) and the incorporation of this model within a CFD simulation framework has been presented. Due to the significant reduction in computational expense, there is potential to extend this approach to substantially more bubbles than is feasible for current DNS approaches, whilst resolving smaller scale flow details than the Euler-Euler and Euler-Lagrange approaches. This study therefore proves a novel concept with the significant potential for expansion.
References


Becker, K., 2002. Perspectives on CFD. In: DGLR Jahrbuch. 6


Bond, W. N., Newton, D. A., 1928. Philosophical Magazine 5, 794–800. 25


Boussinesq, V. J., 1885. Sur la resistance qu’oppose un liquide indefini en repos... C. R. Acad. Sci. 100, 935–937. 29


REFERENCES


Cheung, S. C. P., Yeoh, G. H., Tu, J. Y., 2008. Population balance modeling of bubbly flows considering the hydrodynamics and thermomechanical processes. American Institute of Chemical Engineers. 41


Coetzee, W., Coetzer, R. J. L., Rawatlal, R., 2012a. Response surface strategies in constructing statistical bubble flow models for the development of a novel
bubble column simulation approach. Computers & Chemical Engineering 36, 22–34. 101


Diggle, P. J., 2007. Model-based Geostatistics. Springer. 49, 64


Ekambara, K., Dhotre, M. T., Joshi, J. B., 2005. CFD simulations of bubble column reactors: 1d, 2d and 3d approach. Chemical Engineering Science 60, 6733–6746. 8, 9


Grace, J. R., 1973. Shape and velocities of bubbles rising in infinite liquids. Chemical Engineering Research and Design 51, 116–120. 21


REFERENCES


Lo, S., 1996. Application of musig model to bubbly flows. AEA-Technology AEAT-1096. 40


MATLAB, 2011. version 7.12.0 (R2011a). 125, 137


Perić, M., Bertram, V., 2011. Trends in industry applications of cfd for maritime flows. In: 10th International Conference on Computer and IT Applications in the Maritime Industries. 6


REFERENCES


Saito, S., 1913. On the shape of the nearly spherical drop which falls through a viscous fluid. The Science Reports of Tôhoku Imperial University 2, 179–201. 22


Stokes, G. G., 1851. On the effect of the internal friction of fluids on the motion of a pendulum. Transactions of the Cambridge Philosophical Society 9, 8–106. 20, 29, 84


Leonardo da Vinci, Corbis 1996. CD-ROM. ix, 3, 4

REFERENCES


Ueyama, K., Miyauchi, T., 1979. Properties of recirculating turbulent two-phase flow in gas bubble columns. American Institute of Chemical Engineers 25, 258–266. 31


Wu, M., Gharib, M., 2002. Experimental studies on the shape and path of small air bubbles rising in clean water. Physics of Fluids 14, 49–52. 20


Yang, D., Peterson, D., Li, H., 2012. Compressed sensing and cholesky decomposition on FPGAs and GPUs. Parallel Computing 38, 421–437. 79

Part IV

Appendices
Appendix A

Analytical derivation

The derivation of the velocity equations for the creeping flow past a free-slip sphere is presented here. This derivation is based upon the no-slip solution presented by Slattery [1999].

The velocity components may be written in terms of the Stokes stream function ($\psi$):

$$u_r = \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta} \quad (A.1)$$

$$u_\theta = -\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial r} \quad (A.2)$$

The Navier-Stokes equation simplified for steady-state creeping flow simplifies considerably when written in terms of the stream function.

$$\left[ \frac{\partial^2}{\partial r^2} + \frac{\sin \theta}{r^2} \frac{\partial}{\partial \theta} \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \right) \right]^2 \psi = 0 \quad (A.3)$$

The boundary conditions are:
at \( r = R \)

\[
\begin{align*}
  u_r &= 0 \\
  \frac{\partial u_\theta}{\partial r} &= 0
\end{align*}
\] (A.4)

and at \( r = \infty \)

\[
  u_r = u_\infty \cos \theta
\] (A.6)

The stream function \( \psi \) is arbitrary to a constant and we are free to require as \( r \to \infty \) for \( \theta = 0 \) that \( \psi \to 0 \). This allows as \( r \to \infty \):

\[
\begin{align*}
  \psi &= \int_0^\psi d\psi \\
  &= \int_0^\theta \frac{\partial \psi}{\partial \theta} d\theta \\
  \rightarrow r^2 u_\infty \int_0^\theta \sin \theta \cos \theta d\theta \\
  \rightarrow \frac{1}{2} r^2 u_\infty \sin^2 \theta
\end{align*}
\] (A.8)

The form of the boundary condition suggests a possible form for the stream function of:

\[
  \psi = f(r) \sin^2 \theta
\] (A.11)

With this transformation, the governing equations (Eq. A.3) can be written as:

\[
\frac{d^4 f}{dr^4} - \frac{4}{r^2} \frac{d^2 f}{dr^2} + \frac{8}{r^3} \frac{df}{dr} - \frac{8f}{r^4} = 0
\] (A.12)

The boundary conditions (Eq. A.4 to A.6) can now be written as:
at \( r = R \)

\[
f = 0 \quad \text{(A.13)}
\]

\[
-\frac{1}{R} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} = 0 \quad \text{(A.14)}
\]

and at \( r \to \infty \):

\[
f \to \frac{1}{2} r^2 u_\infty \quad \text{(A.15)}
\]

The fourth-order differential equation (Eq. A.12) is linear and homogeneous. One form of solution is:

\[
f(r) = ar^n \quad \text{(A.16)}
\]

This implies:

\[
f(r) = \frac{A}{r} + Br + Cr^2 + Dr^4 \quad \text{(A.17)}
\]

By substitution of the boundary conditions the coefficients can be found:

\[
A = -\frac{1}{8} u_\infty R^3 \quad \text{(A.18)}
\]

\[
B = -\frac{3}{8} u_\infty R \quad \text{(A.19)}
\]

\[
C = \frac{1}{2} u_\infty \quad \text{(A.20)}
\]

\[
D = 0 \quad \text{(A.21)}
\]

which upon back substitution into Eq. A.1, A.2, A.11 and A.17 yields:

\[
u_r = u_\infty \cos \theta \left[ 1 - \frac{3}{4} \left( \frac{R}{r} \right) - \frac{1}{4} \left( \frac{R}{r} \right)^3 \right] \quad \text{(A.22)}
\]

\[
u_\theta = -u_\infty \sin \theta \left[ 1 - \frac{3}{8} \left( \frac{R}{r} \right) + \frac{1}{8} \left( \frac{R}{r} \right)^3 \right] \quad \text{(A.23)}
\]
Appendix B

Data tables

Table B.1: Fitting Results for surface Re = 0.1 (results from Chapter 4)

<table>
<thead>
<tr>
<th>corr (n_{samp})</th>
<th>RND</th>
<th>LHD</th>
<th>UDC</th>
<th>UPD</th>
<th>UTM</th>
<th>CPD-L</th>
<th>CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp:30</td>
<td>1.47E-011</td>
<td>1.64E-011</td>
<td>5.08E-012</td>
<td>8.91E-012</td>
<td>7.60E-012</td>
<td>7.70E-012</td>
<td>2.08E-012</td>
</tr>
<tr>
<td>exp:60</td>
<td>2.26E-012</td>
<td>2.68E-012</td>
<td>2.89E-012</td>
<td>7.70E-013</td>
<td>1.45E-012</td>
<td>4.50E-012</td>
<td>1.41E-012</td>
</tr>
<tr>
<td>exp:90</td>
<td>1.10E-012</td>
<td>8.74E-013</td>
<td>7.39E-013</td>
<td>1.06E-012</td>
<td>4.96E-013</td>
<td>1.43E-012</td>
<td>1.18E-012</td>
</tr>
<tr>
<td>exp-c:30</td>
<td>1.41E-011</td>
<td>1.46E-011</td>
<td>5.08E-012</td>
<td>3.7E-012</td>
<td>6.77E-012</td>
<td>1.17E-012</td>
<td>1.11E-012</td>
</tr>
<tr>
<td>exp-c:60</td>
<td>2.14E-012</td>
<td>3.05E-012</td>
<td>1.81E-012</td>
<td>1.45E-013</td>
<td>8.22E-013</td>
<td>5.98E-013</td>
<td>2.35E-013</td>
</tr>
<tr>
<td>matern:60</td>
<td>9.82E-012</td>
<td>5.79E-012</td>
<td>6.80E-012</td>
<td>2.36E-012</td>
<td>2.40E-012</td>
<td>1.63E-011</td>
<td>3.91E-012</td>
</tr>
<tr>
<td>matern:90</td>
<td>4.37E-012</td>
<td>2.32E-012</td>
<td>2.33E-012</td>
<td>6.82E-012</td>
<td>1.61E-012</td>
<td>5.12E-012</td>
<td>3.11E-012</td>
</tr>
</tbody>
</table>

* Design and correlation function are not compatible

Table B.2: Fitting Results for surface Re = 15 (results from Chapter 4)

<table>
<thead>
<tr>
<th>corr (n_{samp})</th>
<th>RND</th>
<th>LHD</th>
<th>UDC</th>
<th>UPD</th>
<th>UTM</th>
<th>CPD-L</th>
<th>CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp:30</td>
<td>1.03E-006</td>
<td>1.14E-006</td>
<td>7.22E-007</td>
<td>9.4E-007</td>
<td>1.48E-006</td>
<td>3.02E-006</td>
<td>8.15E-007</td>
</tr>
<tr>
<td>exp:60</td>
<td>3.52E-007</td>
<td>5.47E-007</td>
<td>4.19E-007</td>
<td>1.32E-007</td>
<td>3.51E-007</td>
<td>2.05E-006</td>
<td>2.36E-007</td>
</tr>
<tr>
<td>exp:90</td>
<td>2.32E-007</td>
<td>2.74E-007</td>
<td>1.59E-007</td>
<td>1.60E-007</td>
<td>2.18E-007</td>
<td>2.14E-006</td>
<td>9.74E-008</td>
</tr>
<tr>
<td>exp-c:30</td>
<td>2.47E-006</td>
<td>1.63E-006</td>
<td>7.21E-007</td>
<td>5.82E-007</td>
<td>1.11E-006</td>
<td>2.46E-006</td>
<td>3.45E-007</td>
</tr>
<tr>
<td>exp-c:60</td>
<td>7.07E-007</td>
<td>3.57E-007</td>
<td>3.77E-007</td>
<td>4.58E-008</td>
<td>2.96E-007</td>
<td>1.83E-006</td>
<td>1.08E-007</td>
</tr>
<tr>
<td>exp-c:90</td>
<td>2.76E-007</td>
<td>1.93E-007</td>
<td>1.18E-007</td>
<td>3.79E-008</td>
<td>1.49E-007</td>
<td>1.53E-006</td>
<td>3.50E-008</td>
</tr>
<tr>
<td>matern:30</td>
<td>1.42E-006</td>
<td>1.55E-006</td>
<td>1.15E-006</td>
<td>1.76E-006</td>
<td>3.13E-006</td>
<td>4.15E-006</td>
<td>8.43E-007</td>
</tr>
<tr>
<td>matern:60</td>
<td>8.91E-007</td>
<td>1.86E-006</td>
<td>9.12E-007</td>
<td>3.72E-007</td>
<td>-</td>
<td>4.35E-007</td>
<td>3.24E-006</td>
</tr>
<tr>
<td>matern:90</td>
<td>4.15E-007</td>
<td>1.43E-006</td>
<td>3.72E-007</td>
<td>8.60E-007</td>
<td>3.28E-007</td>
<td>1.42E-006</td>
<td>2.08E-007</td>
</tr>
</tbody>
</table>

* Design and correlation function are not compatible
Table B.3: Fitting Results for surface Re = 75 (results from Chapter 4)

<table>
<thead>
<tr>
<th>corr</th>
<th>samp</th>
<th>RND</th>
<th>LHD</th>
<th>UDC</th>
<th>UPD</th>
<th>UTM</th>
<th>CPD-L</th>
<th>CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp:30</td>
<td>7.16E-005</td>
<td>6.74E-005</td>
<td>2.57E-005</td>
<td>3.78E-005</td>
<td>7.05E-005</td>
<td>1.50E-005</td>
<td>1.65E-005</td>
<td>4.33E-006</td>
</tr>
<tr>
<td>exp:60</td>
<td>2.46E-005</td>
<td>3.66E-005</td>
<td>4.03E-005</td>
<td>7.87E-006</td>
<td>2.50E-005</td>
<td>4.53E-005</td>
<td>8.18E-006</td>
<td></td>
</tr>
<tr>
<td>exp:90</td>
<td>2.72E-005</td>
<td>1.79E-005</td>
<td>1.46E-005</td>
<td>7.33E-006</td>
<td>1.50E-005</td>
<td>1.65E-005</td>
<td>4.33E-006</td>
<td></td>
</tr>
<tr>
<td>exp-c:30</td>
<td>6.09E-005</td>
<td>4.54E-005</td>
<td>2.47E-005</td>
<td>2.99E-005</td>
<td>6.90E-005</td>
<td>3.38E-005</td>
<td>1.99E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:60</td>
<td>3.12E-005</td>
<td>3.92E-005</td>
<td>3.69E-005</td>
<td>3.97E-006</td>
<td>2.04E-005</td>
<td>3.01E-005</td>
<td>5.71E-006</td>
<td></td>
</tr>
<tr>
<td>exp-c:90</td>
<td>2.27E-005</td>
<td>1.79E-005</td>
<td>1.46E-005</td>
<td>7.33E-006</td>
<td>1.36E-005</td>
<td>1.18E-005</td>
<td>3.69E-006</td>
<td></td>
</tr>
<tr>
<td>matern:30</td>
<td>9.55E-005</td>
<td>1.01E-004</td>
<td>3.57E-005</td>
<td>4.54E-005</td>
<td>1.27E-005</td>
<td>5.45E-005</td>
<td>2.62E-005</td>
<td></td>
</tr>
<tr>
<td>matern:60</td>
<td>2.83E-005</td>
<td>2.99E-005</td>
<td>2.04E-005</td>
<td>1.33E-005</td>
<td>2.29E-005</td>
<td>3.16E-005</td>
<td>8.79E-006</td>
<td></td>
</tr>
</tbody>
</table>

* Design and correlation function are not compatible

Table B.4: Fitting Results for surface Re = 135 (results from Chapter 4)

<table>
<thead>
<tr>
<th>corr</th>
<th>samp</th>
<th>RND</th>
<th>LHD</th>
<th>UDC</th>
<th>UPD</th>
<th>UTM</th>
<th>CPD-L</th>
<th>CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp:30</td>
<td>1.26E-004</td>
<td>1.79E-004</td>
<td>1.06E-004</td>
<td>1.16E-004</td>
<td>2.74E-004</td>
<td>1.14E-004</td>
<td>8.20E-005</td>
<td></td>
</tr>
<tr>
<td>exp:60</td>
<td>1.07E-004</td>
<td>1.08E-004</td>
<td>1.98E-004</td>
<td>3.30E-005</td>
<td>1.04E-004</td>
<td>1.13E-004</td>
<td>2.62E-005</td>
<td></td>
</tr>
<tr>
<td>exp:90</td>
<td>8.11E-005</td>
<td>8.11E-005</td>
<td>7.37E-005</td>
<td>3.24E-005</td>
<td>6.30E-005</td>
<td>8.99E-005</td>
<td>1.39E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:30</td>
<td>3.41E-004</td>
<td>1.60E-004</td>
<td>1.03E-004</td>
<td>9.74E-005</td>
<td>2.86E-004</td>
<td>7.98E-005</td>
<td>6.88E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:60</td>
<td>1.36E-004</td>
<td>1.58E-004</td>
<td>1.86E-004</td>
<td>1.91E-005</td>
<td>8.68E-005</td>
<td>7.77E-005</td>
<td>1.81E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:90</td>
<td>6.86E-005</td>
<td>4.38E-005</td>
<td>6.52E-005</td>
<td>1.57E-005</td>
<td>5.22E-005</td>
<td>6.21E-005</td>
<td>9.18E-006</td>
<td></td>
</tr>
<tr>
<td>matern:30</td>
<td>2.58E-004</td>
<td>1.48E-004</td>
<td>1.59E-004</td>
<td>1.21E-004</td>
<td>4.74E-004</td>
<td>1.27E-004</td>
<td>9.56E-005</td>
<td></td>
</tr>
<tr>
<td>matern:60</td>
<td>2.50E-004</td>
<td>1.81E-004</td>
<td>2.38E-004</td>
<td>-</td>
<td>1.28E-004</td>
<td>1.25E-004</td>
<td>4.82E-005</td>
<td></td>
</tr>
<tr>
<td>matern:90</td>
<td>2.98E-004</td>
<td>1.32E-004</td>
<td>1.03E-004</td>
<td>4.33E-005</td>
<td>9.35E-005</td>
<td>1.02E-004</td>
<td>2.72E-005</td>
<td></td>
</tr>
</tbody>
</table>

* Design and correlation function are not compatible

Table B.5: Fitting Results for surface Re = 270 (results from Chapter 4)

<table>
<thead>
<tr>
<th>corr</th>
<th>samp</th>
<th>RND</th>
<th>LHD</th>
<th>UDC</th>
<th>UPD</th>
<th>UTM</th>
<th>CPD-L</th>
<th>CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp:30</td>
<td>9.78E-004</td>
<td>1.24E-003</td>
<td>7.44E-004</td>
<td>4.23E-004</td>
<td>1.26E-003</td>
<td>5.31E-004</td>
<td>3.49E-004</td>
<td></td>
</tr>
<tr>
<td>exp:60</td>
<td>4.99E-004</td>
<td>5.30E-004</td>
<td>1.02E-003</td>
<td>1.50E-004</td>
<td>5.21E-004</td>
<td>4.17E-004</td>
<td>1.17E-004</td>
<td></td>
</tr>
<tr>
<td>exp:90</td>
<td>5.02E-004</td>
<td>2.84E-004</td>
<td>4.17E-004</td>
<td>1.49E-004</td>
<td>3.66E-004</td>
<td>2.49E-004</td>
<td>6.50E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:30</td>
<td>8.17E-004</td>
<td>7.13E-004</td>
<td>7.34E-004</td>
<td>3.21E-004</td>
<td>1.79E-003</td>
<td>1.55E-003</td>
<td>3.43E-004</td>
<td></td>
</tr>
<tr>
<td>exp-c:60</td>
<td>7.34E-004</td>
<td>7.32E-004</td>
<td>9.79E-004</td>
<td>1.29E-004</td>
<td>4.42E-004</td>
<td>3.26E-004</td>
<td>7.28E-005</td>
<td></td>
</tr>
<tr>
<td>exp-c:90</td>
<td>2.81E-004</td>
<td>2.15E-004</td>
<td>3.99E-004</td>
<td>9.30E-005</td>
<td>2.76E-004</td>
<td>3.39E-004</td>
<td>5.11E-005</td>
<td></td>
</tr>
<tr>
<td>matern:30</td>
<td>1.36E-003</td>
<td>1.61E-003</td>
<td>7.91E-004</td>
<td>4.12E-004</td>
<td>2.06E-003</td>
<td>4.91E-004</td>
<td>3.67E-004</td>
<td></td>
</tr>
<tr>
<td>matern:60</td>
<td>1.30E-003</td>
<td>7.20E-004</td>
<td>1.15E-003</td>
<td>-</td>
<td>6.43E-004</td>
<td>4.41E-004</td>
<td>1.34E-004</td>
<td></td>
</tr>
<tr>
<td>matern:90</td>
<td>4.43E-004</td>
<td>3.27E-004</td>
<td>5.49E-004</td>
<td>1.86E-004</td>
<td>4.28E-004</td>
<td>3.28E-004</td>
<td>1.13E-004</td>
<td></td>
</tr>
</tbody>
</table>

* Design and correlation function are not compatible
Table B.6: Fitting Results for surface SRD (results from Chapter 4)

<table>
<thead>
<tr>
<th>Run/Temp</th>
<th>SRD</th>
<th>SRD+UDC</th>
<th>SRD+UDP</th>
<th>SRD+UTM</th>
<th>SRD+CPD-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1:30</td>
<td>9.87E-013</td>
<td>2.10E-012</td>
<td>3.48E-012</td>
<td>8.30E-013</td>
<td>1.41E-012</td>
</tr>
<tr>
<td>0.1:90</td>
<td>7.79E-014</td>
<td>1.62E-013</td>
<td>1.55E-013</td>
<td>7.89E-014</td>
<td>2.26E-013</td>
</tr>
<tr>
<td>15:30</td>
<td>5.68E-007</td>
<td>2.84E-007</td>
<td>6.27E-007</td>
<td>2.52E-007</td>
<td>3.80E-007</td>
</tr>
<tr>
<td>15:60</td>
<td>3.72E-008</td>
<td>4.90E-008</td>
<td>9.32E-008</td>
<td>6.94E-008</td>
<td>1.89E-007</td>
</tr>
<tr>
<td>15:90</td>
<td>1.33E-008</td>
<td>1.81E-008</td>
<td>3.08E-008</td>
<td>1.87E-008</td>
<td>5.28E-008</td>
</tr>
<tr>
<td>75:30</td>
<td>1.24E-005</td>
<td>9.73E-006</td>
<td>1.53E-005</td>
<td>1.19E-005</td>
<td>2.73E-005</td>
</tr>
<tr>
<td>75:60</td>
<td>1.91E-005</td>
<td>4.01E-006</td>
<td>3.94E-006</td>
<td>3.96E-006</td>
<td>6.31E-006</td>
</tr>
<tr>
<td>75:90</td>
<td>1.80E-005</td>
<td>1.60E-006</td>
<td>1.93E-006</td>
<td>1.46E-006</td>
<td>1.40E-006</td>
</tr>
<tr>
<td>135:30</td>
<td>4.55E-005</td>
<td>4.04E-005</td>
<td>4.09E-005</td>
<td>3.69E-005</td>
<td>1.48E-004</td>
</tr>
<tr>
<td>135:60</td>
<td>4.43E-005</td>
<td>1.50E-005</td>
<td>1.85E-005</td>
<td>1.28E-005</td>
<td>1.17E-005</td>
</tr>
<tr>
<td>270:30</td>
<td>1.85E-004</td>
<td>1.82E-004</td>
<td>1.42E-004</td>
<td>1.61E-004</td>
<td>3.73E-004</td>
</tr>
<tr>
<td>270:60</td>
<td>6.51E-005</td>
<td>5.56E-005</td>
<td>1.01E-004</td>
<td>5.18E-005</td>
<td>1.03E-004</td>
</tr>
<tr>
<td>270:90</td>
<td>3.27E-005</td>
<td>2.4E-005</td>
<td>4.42E-005</td>
<td>2.31E-005</td>
<td>2.94E-005</td>
</tr>
</tbody>
</table>
Appendix C

Computer code

```cpp
void Foam::solidParticle::cellsOccupied(labelList& cellsOcc, labelList& cellsPerParticle, labelList& fsCells, labelList& fsCellsPP, const vector& cellL, const vector& meshR, const fvMesh& mesh)
{
    scalar regionRatio = 5.0;
    scalar regionRadius = regionRatio*d_/2.0;
    label pO = cell();
    label pO2(pO), pO3(pO), pO4(pO), pOn(pO), pO2n(pO);

    Info << "cell: " << cell() << endl;

    int nCells;

    {
        nCells = round(((PI*regionRadius*regionRadius)/(cellL[0]*cellL[1]*cellL[2])));
    }
    else
    {
        nCells = round(((4.0/3.0)*PI*regionRadius*regionRadius*regionRadius*regionRadius)/(cellL[0]*cellL[1]*cellL[2]));
    }

    labelList cellSet(nCells);

    int n_y = ceil(regionRadius/cellL[1]);
    int n_z = ceil(regionRadius/cellL[2]);

    scalar yc, zc, x1, n_x;
```
int count = 0;
for (int ii=0;ii<n_z;ii++)
{
    zc = ii*cellL[2];
    for (int jj=0;jj<n_y;jj++)
    {
        yc = jj*cellL[1];
        xl = regionRadius*regionRadius - yc*yc - zc*zc;
        if (xl >0) { n_x = round(sqrt(xl)/cellL[0]);}
        else { n_x = 0;}
    }
    for (int kk=0;kk<n_x;kk++)
    {
        cellSet[count] = pO+kk; count ++;
        if (kk >0) { cellSet[count] = pO-kk; count ++;}
        if (pO != pO2)
        {
            cellSet[count] = pO2+kk; count ++;
            if (kk >0) { cellSet[count] = pO2-kk; count ++;}
        }
    }
}
if (ii>0)
{
    cellSet[count] = pOn+kk; count ++;
    if (kk>0) { cellSet[count] = pOn-kk; count ++;}
    if (pOn != pO2n)
    {
        cellSet[count] = pO2n+kk; count ++;
        if (kk>0) { cellSet[count] = pO2n-kk; count ++;}
    }
}
}
}

p0 += meshR[0]; p02 -= meshR[0];
p0n += meshR[0]; p02n -= meshR[0];
p03 += meshR[0]*meshR[1];
p04 -= meshR[0]*meshR[1];
p0 = p03; p02 = p03;
p0n = p04; p02n = p04;

labelList cellSetF(count);
for (int ii=0;ii<count;ii++) { cellSetF[ii] = cellSet[ii];}

int countS(0), countFS(0);
p0 = cell();
vector xc1, xc2, xc;
// 2-ellipsoid parameters
scalar xzMult = 1.25;
scalar ypMult = 2.0;

// compute angles of bubble velocity vector
scalar t_ax = Foam::atan2(Us_[2], Us_[1]);
scalar t_az = -Foam::atan2(Us_[0], Foam::sqrt(Us_[1]*Us_[1] + Us_[2]*Us_[2]));

// construct rotation matrices
tensor rX1(1.0,0.0,0.0,0.0,Foam::cos(-t_ax),-Foam::sin(-t_ax),0.0,Foam::sin(-t_ax),Foam::cos(-t_ax));
tensor rZ1(Foam::cos(-t_az),-Foam::sin(-t_az),0.0,Foam::sin(-t_az),Foam::cos(-t_az),0.0,0.0,0.0,1.0);

for (int ii = 0; ii < count; ii++)
{
    xc1 = mesh.C()[cellSetF[ii]] - mesh.C()[pO];
    xc2 = rX1 & xc1;
    xc = rZ1 & xc2;
    if ((xc[1] >= 0.0) && (powf(powf(ypMult*xc[1],2.0) + powf(xzMult*fabs(xc[0]),2.0) + powf(xzMult*fabs(xc[2]),2.0),0.5) < 5.0*d_/2.0))
        { cellsOcc_.append(cellSetF[ii]); countS++; };
    if ((xc[1] < 0.0) && (powf(powf(xc[1],2.0) + powf(xzMult*fabs(xc[0]),2.0) + powf(xzMult*fabs(xc[2]),2.0),0.5) < 5.0*d_/2.0))
        { cellsOcc_.append(cellSetF[ii]); countS++; };

    // free stream cells
    if ((xc[1] > 0.0) && (powf(powf(ypMult*xc[1],2.0) + powf(xzMult*fabs(xc[0]),2.0) + powf(xzMult*fabs(xc[2]),2.0),0.5) > 5.0*d_/2.0))
        { fsCells_.append(cellSetF[ii]); countFS++; };
}

labelList cPP(1), fcPP(1);
cPP = countS; fcPP = countFS;

cellsPerParticle_.append(cPP);
Info<<"n_cells : "<<countS<<endl;
fsCellsPP_.append(fcPP);

1 void Foam::solidParticle::getBCMVelocities(const labelList& cellsOcc, const labelList& cellsPerParticle, vectorField& uVal, scalarField& pVal, const
fvMesh & mesh, const int & count, const scalar urP[], const scalar utP[],
const scalar pP[], const volVectorField & Ugrid)
{
    Info<<"Particle Number : " <<count <<nl << endl ;
    Info<<"Reynolds number : " <<Re_ <<nl << endl ;
    // Fluid properties "_o" are used for scaling purposes
    scalar u_inf = mag(Us_);
    scalar mu_o (0.001003); // kg/m.s
    scalar rho_o (998.2); // kg/m3
    scalar R_o (0.0005); // m
    scalar R = d_/2.0;
    scalar scX = 7.663075740482863e-04*(R/R_o);
    scalar scR = Re_ * mu_o /(2.0* rho_o * R_o * u_inf);
    scalar scU = -u_inf * scR;
    vector Usc = U_ - Us_;

    // compute first stage coefficients using second stage models


    // compute angles of bubble velocity vector
    scalar t_ax = Foam::atan2(Us_[2],Us_[1]);
    scalar t_az = -Foam::atan2(Us_[1]*Us_[1] + Us_[2]*Us_[2]);
    // construct rotation matrices
    tensor rX(1.0,0.0,0.0,0.0,0.0,0.0);Foam::cos(t_ax),-Foam::sin(t_ax),0.0,Foam::sin(t_ax),Foam::cos(t_ax));
    tensor rZ(Foam::cos(t_az),-Foam::sin(t_az),0.0,Foam::sin(t_az),Foam::cos(t_az),0.0,0.0,0.0,1.0);
    tensor rX1(1.0,0.0,0.0,0.0,0.0,0.0,Foam::cos(-t_ax),-Foam::sin(-t_ax),0.0,Foam::sin(-t_ax),Foam::cos(-t_ax));
tensor rZ1(Foam::cos(-t_az),-Foam::sin(-t_az),0.0,Foam::sin(-t_az),Foam::cos
(-t_az),0.0,0.0,0.0,1.0);

vector x, xr1, uv1, uv2, uv3;
scalar r, rm, phi, tm, tmh;
scalar ut, ur, uax;
scalar tr1, tr2, tr3, pm;
int nCells = cellsPerParticle[count-1];
vectorField ucc(nCells);
scalarField pcc(nCells);

scalar yExit = mesh.C()[Ugrid.size()-1][1] + mesh.C()[0][1];
Info<<"cellsPerParticle: "<<nCells<<endl;
int occAdd(0);
for (int ii=0; ii<(count-1);ii++) {occAdd += cellsPerParticle[ii];}
//scalar occAdd = (count-1)*nCells;
Info<<"occAdd: "<<occAdd<<endl;

for (int ii=0; ii<nCells;ii++)
{
  x = mesh.C()[cellsOcc[occAdd+ii]] - mesh.C()[cell()];
xr1 = rX1 & x;
x = rZ1 & xr1;

  r = mag(x);
  phi = Foam::atan2(x[2],x[0]);
  rm = r/scX;
  tm = Foam::atan2(Foam::sqrt(x[0]*x[0]+x[2]*x[2]),x[1]);
  tmh = ceil((sign(tm-alp[16]) / alp[16])*(tm-alp[16]) + alp[16]);
  if ( r > 1.0001*R )
  {
    // radial velocity models
    act = ceil(sign(alp[16]-tm)/alp[16]);
    ur_A = ur_fa(alp[0],alp[1],scU/alp[17],R/scX,rm,tm);
    ur_S = ur_fs(alp[2],alp[3],alp[4],alp[5],alp[6],alp[7],alp[8],alp
               [9],alp[10],alp[11],alp[12],alp[13],alp[14],alp[15],alp[16],rm,
               tm,tmh,act);
    // angular velocity models
    ut_A = ut_fa(alp[0],alp[1],scU/alp[9],R/scX,rm,tm);
    ut_S = ut_fs(alp[2],alp[3],alp[4],alp[5],alp[6],alp[7],alp[8],R/scX,
                 rm,tm);
    // combined velocity models
    ur = alp[17]*(ur_A+ur_S);
    ut = alp[9]*(ut_A+ut_S);
    // convert to cartesian velocities
    uax = ur*Foam::sin(tm)+ut*Foam::cos(tm);
uv1[0] = Foam::cos(phi)*uax/scR;
uv1[1] = (ur*Foam::cos(tm) - ut*Foam::sin(tm))/scR + u_inf;
uv1[2] = Foam::sin(phi)*uax/scR;
  // rotate according to direction vector
uv2 = rZ & uv1;
uv3 = rX & uv2;
uv3 = uv3 + Usc*powf(R/r,1.0);
  // condition to not simply overwrite when BCM velocity is very small
  and other velocity exists
if ((3.0*mag(uv3))>mag(Ugrid[cellsOcc[occAdd+ii]]))
  {ucc[ii] = uv3;}
else {ucc[ii] = Ugrid[cellsOcc[occAdd+ii]];};
pcc[ii] = 9.81*(yExit-mesh.C()[cellsOcc[occAdd+ii]][1]);
}
else
{
  ucc[ii] = {0.0,0.0,0.0};
pcc[ii] = 9.81*(yExit-mesh.C()[cellsOcc[occAdd+ii]][1]);
};

uVal.append(ucc);
pVal.append(pcc);