USING DIRECT NUMERICAL SIMULATION AND STATISTICAL LEARNING
TO MODEL BUBBLY FLOWS IN VERTICAL CHANNELS

A Dissertation

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Abstract

by

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Direct Numerical Simulations (DNS) of multiphase flows have progressed rapidly over the last decade and it is now possible to simulate motions of hundreds of deformable bubbles in turbulent flows. The availability of different statistics calculated from such DNS data could help advance the development of new reduced order models of the average or large-scale flows.

DNS simulation of a laminar system with nearly spherical bubbles have been used to examine the full transient motion and shows a non-monotonic evolution where all the bubbles first move toward the walls and then the liquid slows down, eventually allowing some bubbles to return to the center of the channel. DNS simulation of a turbulent system with bubbles of different sizes at a friction Reynolds number of 250 shows that small bubbles quickly migrate to the wall, but the bulk flow takes much longer to adjust to the new bubble distribution.

The DNS results are then used to help develop the averaged model equations with unknown closures accounting for the effect of the unresolved scales. A database is generated by averaging the DNS results over planes parallel to the stream-wise direction of the flow. The most important turbulent quantities are selected first with the feature selection algorithm. Then a Neural Network (NN) is used for the a priori test, to examine the relationships between unknown closure terms in averaged models.
for the flow and quantities that are available through the DNS results. For laminar cases, the closure relations are then tested, by following the evolution of different initial conditions, and it is found that the model predictions are in reasonably good agreement with DNS results. For turbulent cases, the preliminary results for the feature selection and a priori test are promising and robust, the future work is to validate the predictive performance of the turbulent modeling.
To my dearest mother Wu Gongmei and father Ma Xinhua
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CHAPTER 1

GENERAL INTRODUCTION

1.1 Motivation

Direct numerical simulations (DNS) of multiphase flows, where every continuum length and time scale are fully resolved, are starting to provide new insights into various aspects of the dynamics of such flows [Esmaeeli and Tryggvason, 2005, Lu and Tryggvason, 2013, van Sint Annaland et al., 2006]. For many multiphase flows the physics is well understood in the sense that the dynamics is believed to be accurately described by the Navier-Stokes equations, but for most flows of industrial interest DNS require too fine grid resolution to be practical on current computers. Furthermore, since the small scale behavior often exhibits significant universality, it is likely that in many cases the small scales can be modeled, rather than fully resolved. One emerging challenge is therefore how to take advantage of DNS results to generate reliable, reduced order model at industrial scale, where DNS is not practical.

For many purposes a low order description of the system, such as the average motion, is all that is needed. A reduced order description can be derived by averaging or filtering the Navier-Stokes equations, but the process introduces unknown closure terms that account for the effect of the unresolved scales on the resolved ones. Those have to be modeled. The fundamental assumption behind modeling of multiphase flows is that the closure terms appearing in the equations for the averaged or filtered quantities depend on the averaged flow, such as the deformation tensor and the void fraction, and sometimes on some integral measures of the unresolved motion, such
as the turbulent kinetic energy, dissipation rate, and surface area density. The latter quantities evolve by their own equations with their own closure terms that need to be related to other quantities, in the same way as for the equations for the average flow. The averaged and filtered equations can be written in several different forms and depending on the exact form we need different closure relations.

In the current work, we have explored the feature selection methods to select the most important features in the system, which act as the dependent variables of the unknown closures. Then the Neural Networks (NN) and linear regression are used to obtain the closure relations for the two-fluid equations for the average motion of bubbly flows, by mining DNS results. For laminar cases, we follow the evolution of one initial bubble distribution and velocity profile using DNS and then fit the data to produce the closure relations for the equations for the average flow. The model is then used to predict the evolution of other initial conditions for validation tests. For turbulent cases, we are still focused on the feature selection and a priori test, similar prediction works discussed in the laminar system will be explored and finally applied to the turbulent system in the future.

1.2 Literature review

For single phase flows, DNS have resulted in significant progress in modeling unresolved scales, including how they depend on the large scale resolved flow and how the small scales in turn influence the larger scales. Developments of new models have, in particular, lead to new questions that have motivated new simulations.

Modeling of multiphase flows generally builds on the two-fluid model [Harlow and Amsden, 1975, Ishii, 1975], where separate equations are solved for the average motion of the different fluids. The averaged equations have been examined analytically for laminar bubbly flow by [Antal et al., 1991] and later by [Azpitarte and Buscaglia, 2003]. For turbulent flow [Drew and Lahey, 1993] solved the equations for the average
flow using asymptotic analysis, and numerical solutions have been reported by a number of investigators [Guet et al., 2005, Kuo et al., 1997, Lopez De Bertodano et al., 1987, 1994]. The results, both for laminar and turbulent flows, generally agree with the flow structure seen experimentally, once the model coefficients have been tuned appropriately. For nearly spherical bubbles this includes uniform velocity and void fraction in the core, wall peaking for up-flow and a wall-layer without bubbles for down-flow. The current status of such models has been reviewed by a number of authors [Drew, 1983, Prosperetti and Tryggvason, 2007]. Although DNS of multiphase flows have progressed rapidly during the last two decades, attempts to use DNS results to help modeling of multiphase flows are still rare. The most intense effort appears to have been by a French group, who has published several papers on LES (large eddy simulations) modeling of multiphase flows, including the derivation of the filtered LES equations, identification of the unresolved terms, and comparisons of model results with DNS [E. Labourasse et al., 2007, Toutant et al., 2008, 2009a,b].

Applications of various statistical techniques have a long history in studies of complex flows [Huffman et al., 1973], for example. As the use of such techniques has become more widespread for a large range of other problems, ranging from predicting consumer preferences to identifying security threats, methods for statistical learning have advanced rapidly. For multiphase materials, the use of neural networks to develop reduced order models from simulation data has a history for solid mechanics applications and recent examples include models for damage in concrete [Unger and Kônke, 2008] and bones [Hambli, 2011a,b].

For single phase turbulent modelling, [Milano and Koumoutsakos, 2002] used neural networks to reconstruct near-wall turbulent flows and [Rajabi and Kavianpour, 2012] used neural network to interpolate DNS data for a backward facing step. Other examples includes the development of a subgrid model for LES by [Sarghini et al., 2003], the optimal estimation of subgrid models for LES by [Moreau et al., 2006],
the parametrization of surface features in coarse LES by [Esau and Rieber, 2010], and the use of neural networks to optimize the model constants of the \( k - \varepsilon \) turbulence model applied to simulations of data centers by [Yarlanki et al., 2012]. [Tracey et al., 2015] used statistical learning to determine the functional dependency of the closure terms for data generated by Spalart-Allmaras turbulence model, rather than full DNS. On the other hand, [Duraisamy et al., 2015] and [Parish and Duraisamy, 2016] used inverse modeling to obtain spatially distributed functional terms to aid closure modeling, instead of inferring model parameters directly, and later [Singh, 2016] have used the similar method for turbulent flows over airfoils involving flow separation, showing much improved predictions in lift and surface pressure. In the last couple of years, due to the rapid development of machine learning techniques, increasingly efforts are focused on how to combine machine learning with turbulent modeling and how to generalize the RANS model with machine learning, [Ling, 2016a] specifically addressed physical systems that possess symmetry or invariance properties by comparing two different methods for teaching a machine learning model an invariance property, and shows that embedding the invariance property into the input features yields higher performance with less computational cost. [Ling, 2016b] presents a method of using deep neural networks to learn a model for the Reynolds stress anisotropy tensor from high-fidelity simulation data, demonstrating significant improvement over baseline RANS linear eddy viscosity and nonlinear eddy viscosity models, based on two test cases. [Xiao, 2016] used a random forest regression to predict the discrepancies of RANS turbulent stresses, demonstrating that the discrepancies in the modeled Reynolds stresses can be explained by the mean flow feature. Meanwhile, [Wu, 2016] and [Wang, 2016] have tried to learn the functional form of the Reynolds stress discrepancy in RANS simulations based on available data, and also showed the predictive power of the learned RANS turbulent stress by testing the model on new cases. Unlike using machine learning to improve the RANS model,
[Gamahara, 2016] used neural network (NN) as a tool for exploring a new subgrid model of the subgrid-scale (SGS) stress for large-eddy simulation based on turbulent channel flow DNS database.

For multiphase flows, [Lu et al., 2012] computed the response of fully resolved particles to a shock and used a neural network to develop closure laws for macroscopic simulations of the gas-particle mixture. [Sen et al., 2015] discussed various techniques to bridge the scales between detailed microscopic simulations and macroscopic models, focusing on the convergence rate for various model problems.

Other applications include the use of statistical learning to quantify the uncertainty in model predictions. [Oliver and Moser, 2011] used Bayesian probabilistic approach to quantify the uncertainty in RANS model predictions for turbulent channel flow, [Cheung et al., 2011] examined the uncertainty for turbulent boundary layers, and [Ling and Templeton, 2015] used machine learning to compare RANS results with DNS and LES predictions to identify regions of high uncertainty, presumably where the assumptions behind the RANS model no longer hold. For our purpose, the use of statistical learning to automate, at least partially, the development and evaluation of reduced order models, is most relevant.

In chapter 2, the numerical method, computational settings, and the averaged models are discussed. In chapter 3, we used neural network to obtain closure relationships for laminar bubbly up-flows in fully periodic domains from DNS results and found that the relationships allowed us to predict the evolution of different initial conditions (velocity and void fraction profiles) using a simple two-fluid model for the average flow. This study has been published in [Ma et al., 2015]. In chapter 4, we examined an infinitely long vertical channel with flow driven by an imposed pressure gradient and gravity. The average flow is homogeneous in the stream-wise and span-wise direction and the averaged quantities depend only on the wall-normal coordinate, as well as time. [Ma et al., 2016] discusses these results in details.
For both two scenarios we use DNS results to find closure relationships for the average two-fluid model by model averaging neural networks. Although wall-bounded flow is similar to the one examined in our previous works, the presence of walls adds considerable complexity. Firstly, even though the governing parameters are chosen so that the bubbles remain nearly spherical, surface tension effects are important near the wall and must be included in the average model, resulting in new terms that must be closed. Secondly, finding the neural network coefficients for the relationships between the closure terms and the resolved average variables is much more difficult and we have had to adopt new strategies to train the model. Since the bubbles are driven to the wall relatively quickly at the early stage, but the flow then changes relatively slowly, new data sampling strategies have been used. Those strategies are discussed in the method section.

In the chapter 5, we show that how DNS results can assist turbulent bubbly flow modeling continuing the studies of the laminar flows in previous chapters. The topics include the turbulent feature selection for the unresolved closure terms, a priori test with the DNS data for the NN’s fitting, identification of bubbly wall layer and interior-region, and methods to make a more comprehensive training dataset.
CHAPTER 2

METHODOLOGY

2.1 Numerical method and problem setup

We have examined two scenarios using DNS results. The first geometry is a rectangular box with periodic boundary condition in all three directions, and the other is a rectangular vertical channel, bounded by two parallel vertical plates, as sketched in Figure 2.1. In order to simulate an infinitely long channel, the boundary condition in $y$ direction is periodic. Gravity acts in the negative $y$ direction and the initial average velocity and void fraction depend only on the $x$ coordinate, but not on $y$ or $z$. As the flow evolves, the various averaged quantities are therefore functions of $x$ only.

For fully periodic case, we examine just one set of material parameters and take the liquid density to be $\rho_l = 0.25$, the liquid viscosity to be $\mu_l = 0.008$, and the surface tension to be $\sigma = 0.4$. The bubble density and viscosity are one twentieth of the values for the liquid, or $\rho_g/\rho_l = \mu_g/\mu_l = 0.05$, where the subscript $l$ denotes the liquid and $g$ stands for the gas. The bubbles are all of the same size, with a diameter $d = 0.18$, but their number is varied to give different volume fractions. The gravity acceleration is $g_y = 1$. These parameters result in a Morton number of $M = g_y \mu_l^4/\rho_l \sigma^3 = 2.56 \times 10^{-8}$ and an Eötvös number of $Eo = \rho_l g_y d^3/\sigma = 0.2025$. The domain side is $2.0 \times 1.5 \times 1.0$ computational units in the $x$, $y$, and $z$ direction and the DNS have been done using a $256 \times 192 \times 128$ uniformly spaced grid. Simulations with both finer and coarser grid show that the results are essentially fully converged.
Figure 2.1. A sketch of the computational domain. The domain is bounded by vertical walls (blue planes) and is periodic in the stream-wise y-directions and span-wise z-direction. The gray plane in the middle shows one of the plans where the N-S equation is averaged on.
For the laminar wall-bounded case, the problem specification is similar to the fully periodic case. The width of the domain, in the wall-normal direction is $H = 2$, in the stream-wise direction the length is $L = 1.5$ and the span-wise width is $W = 1.0$. To make the computations as easy as possible, the density and viscosity are taken to be $\rho_l/\rho_g = 2.5/0.125$; and $\mu_l/\mu_g = 0.01/0.005$. Gravity acceleration is $g_y = 1.0$ and total pressure gradient in the stream-wise direction is $\beta = -0.04$, where $\beta = dp_o/dy + \rho_{avg}g_y$. The flow contains $N = 49$ bubbles of diameter $d_e = 0.18$, giving an average void fraction of $\alpha_{avg} = 0.049$. The surface tension coefficient is $\sigma = 0.4$, and these parameters result in a Morton number of $M = g_y\mu_l^4/\rho_l\sigma^3 = 2.56 \times 10^{-8}$ and an Eötvös number of $Eo = \rho_l g_y d^2/\sigma = 0.2025$. The initial velocity is a parabolic profile

$$U(y) = \frac{H^2\beta}{2\mu_l} \left[ \left( \frac{y}{H} \right)^2 - \frac{y}{H} \right], \quad (2.1)$$

where the wall shear balances the pressure gradient and the weight of the mixture. The maximum velocity is $U_{max} = 3.00$, and the bulk velocity of the channel is $U_b = 2.0$. The channel Reynolds number based on the bulk velocity and width of the channel is 1000. The domain is resolved by $192 \times 192 \times 128$ grid points in the stream-wise, wall-normal and span-wise direction. The grid is stretched in the wall-normal direction to increase the resolution at the wall. For further details, see [Lu et al., 2006]. At steady state, the average wall shear stress $\tau_w$ is related to the pressure gradient and the weight of the bubble/liquid mixture by a stream-wise momentum balance:

$$\tau_w = -(dP_0/dz + \rho_{avg}g_y)h = -\beta H/2, \quad (2.2)$$

which is found by taking a simple force balance for the whole domain. Since the liquid and the bubbles are incompressible, $\rho_{avg}$ is constant, and $\beta$ is therefore constant, since we assume that the imposed pressure gradient does not change. The direction of the flow depends directly on the sign of $\beta$ and for upflow we must have $\beta < 0$. 
The drift of the bubbles and its dependency on the independent parameters like the liquid shear rate changes, when the bubbles start to accumulate near the wall. Thus, in the turbulent wall-bounded case, we initially focus on the data from the liquid core region, which is the region more than one bubble diameter away from the wall. We have tried a variety of Reynold number based on half width of the channel, respectively at 6000, 8000 and 9000, together with different shear rate in regions far from the wall and different bubble void fractions as well. The main goal is to increase the parameter ranges for the training data, and learn a more generalized model based on the training data. For the turbulent flows, the width of the domain, in the wall-normal direction is $H = 2$, in the stream-wise direction the length is $L = 6.2832$ and the span-wise width is $W = 1.5708$. The density and viscosity are taken to be $\rho_l/\rho_g = 1.0/0.1$; and $\mu_l/\mu_g = 0.0003333/0.00003333$. Gravity acceleration is $g_y = 0.1361$ and total pressure gradient in the stream-wise direction is $\beta = -0.001799$, similar as in the laminar case where $\beta = dp_o/dy + \rho_{avg}g_y$. The flow contains $N = 30$ bubbles of diameter $d_e = 0.2$. The surface tension coefficient is $\sigma = 0.0544$, and these parameters result in a Morton number of $Mo = g_y\mu_l^4/\rho_l\sigma^3 = 2.56 \times 10^{-10}$ and an Eötvös number of $Eo = \rho_l g_y d^2/\sigma = 0.12$. The initial velocity is a combination of the pressure driving parabolic profile with a moving velocity at the wall. The main goal of using this Couette-Poiseuille (C-P) turbulent flow is to generate a relatively large average liquid shear rate at the channel interior-region.

For the turbulent velocity initialization, we adopt a spectral code package named Channelflow [Gibson, 2014, Gibson et al., 2008], which is a software system for numerical analysis of the incompressible Navier-Stokes flow in channel geometries, written in C++. The Channelflow package is based on a spectral algorithm for integrating the Navier-Stokes equations. Channelflow consists of a software library for a set of predefined executable programs to initialize the liquid turbulent velocity profile to steady state, and greatly saved the computational time during the turbulent initial-
ization. After we get the liquid 3D velocity profile, we interpolate the results to use as initial conditions in our code, add the bubbles, and rerun the simulation again for transient results.

The numerical method for the DNS used for all three scenarios is the same. The Navier-Stokes equations are solved by an explicit projection method that is second order in time, using a fixed, staggered grid where the advection terms are resolved by a QUICK scheme and the viscous terms by a second order centered approximation. In order to keep the boundary between the different fluids sharp, to advect the density and the viscosity fields, and to accurately compute the surface tension, the fluid interface is tracked by connected marker points (the “front”). The front points, which are connected to form an unstructured surface grid, are advected by the fluid velocity, interpolated from the fixed grid. As the front deforms, surface markers are dynamically added and deleted. The surface tension is represented by a distribution of singularities (delta-functions) located at the front. The gradients of the density and viscosity become delta functions when the change is abrupt across the boundary. To transfer the front singularities to the fixed grid, the delta functions are approximated by smoother functions, with a compact support, on the fixed grid. At each time step, after the front has been advected, the density and the viscosity fields are reconstructed by integration of the smooth grid-delta function. The surface tension is then added to the nodal values of the discrete Navier-Stokes equations. Finally, an elliptic pressure equation is solved by a multigrid method to impose a divergence-free velocity field. The method has been applied to several multiluid problems and tested and validated in a number of ways. Those tests include comparisons with analytical solutions for simple problems [Lu et al., 2006], other numerical computations [van Sint Annaland et al., 2006], and experiments [Prosperetti and Tryggvason, 2007]. The actual resolution requirement varies with the governing parameters of the problem and high Reynolds numbers flows, for example, generally require finer resolution
than low Reynolds number flows, as in other numerical calculations, and examples of a detailed description of the method can be found in [Tryggvason et al., 2011].

2.2 Phasic average model

To derive equations for the average void fraction and the average vertical velocity as functions of the wall-normal coordinate, we integrate the mass and momentum equations over planes parallel to the walls, taking the density and the viscosity of the gas to be zero. The details are shown in the appendix. We define the average liquid volume fraction and the average phasic vertical liquid velocity by

\[
\alpha_l = \frac{1}{A_{zy}} \int \chi da, \quad < v >_l = \frac{1}{\alpha_l A_{zy}} \int \chi v da.
\]

where \( \chi \) is an indicator function such that \( \chi = 1 \) in the liquid phase and \( \chi = 0 \) in the gas. \( A_{zy} \) is the area of a plane parallel to the walls, as sketched in Figure 2.1. The results of the averaging are two equations for the liquid volume fraction and the average vertical velocity of the liquid. The equation for the average liquid volume fraction is:

\[
\frac{\partial \alpha_l}{\partial t} + \frac{\partial F_l}{\partial x} = 0,
\]

where the horizontal flux of liquid is given by

\[
F_l = \frac{1}{\alpha_l A_{zy}} \int \chi u da = \alpha_l < u >_l.
\]

The gas volume fraction, \( \alpha_g \), and average horizontal velocity, \( < u >_g \), are found in the same way. Adding the equations for the gas and the liquid, using that the volume fractions must add up to unity, \( \alpha_l + \alpha_g = 1 \), and that the \( u \) velocities at the walls are zero, shows that

\[
F_g + F_l = \alpha_g < u >_g + \alpha_l < u >_l = 0.
\]

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Thus, gas flow in one horizontal direction is always balanced by liquid flow in the opposite direction.

The averaged equation for the vertical liquid velocity \( \langle v \rangle_l \) is:

\[
\frac{\partial}{\partial t} \alpha_l \langle v \rangle_l + \frac{\partial}{\partial x} \alpha_l \langle u \rangle_l \langle v \rangle_l = -\frac{1}{\rho_l} \frac{dp}{dy} \frac{1}{\rho_l \alpha_l g_y} + \frac{1}{\rho_l} \frac{\partial}{\partial x} \left( \alpha_l \mu_l \frac{\partial \langle v \rangle_l}{\partial x} \right) - \frac{\partial}{\partial x} \left( \alpha_l \langle uw \rangle_l \right) + (f_\sigma)_y.
\]

where the last term is the average surface tension. Notice that the momentum equation contains the liquid fluxes since the average horizontal liquid velocity is given by \( \alpha_l \langle u \rangle_l = F_l \). Equations (2.4) and (2.7) give the evolution of \( \alpha_l \) and \( \langle v \rangle_l \), but require closure relations for \( F_l \), \( \langle uw \rangle_l \) and \( (f_\sigma)_y \).

The equations (2.4) and (2.7) are solved by a simple first order finite volume method with sufficiently fine grid and small time steps to ensure that the solution has converged. Since we made a few assumptions in deriving the average equations that are not satisfied exactly by the DNS (such as ignoring the density and viscosity of the gas phase), we have computed each term in the model equations from the DNS data to check how well it is satisfied. The residual (computed as the difference between the left and right hand side) is always less than 8 percentage of the magnitude of left or right hand side.

2.3 Statistical learning for unknown closures

The DNS results contain a detailed description of the flow so that the closure terms in the averaged equations can be calculated at every spatial and temporal location. Thus, we can compute the average velocity, void fraction, and any other quantities of interest. The fundamental assumption behind modeling the average flow is that the closure terms appearing in the model equations depend on the average flow and possibly some integral measures of the unresolved motion. For laminar flows,
we assume that unresolved terms are not needed to model the unknown closures, since all the unsteadiness is due to the motion of the bubbles. However, in turbulent flows, it is essential to include the quantities representing the state of the unresolved turbulent scales.

To develop models for the closure terms, the gas flux $F_g$ (or the average horizontal gas velocity $< u >_g$) the streaming stresses $< u'v' >_l$ and the average surface tension force $(f_\sigma)_y$, we use the results of DNS of one system to “teach” the model how they depend on the average variables. Then we evaluate how good the model is by computing how other initial bubble distribution and velocities evolve and comparing the results with DNS simulations. To keep the development as simple as possible, in the laminar cases we make the rather significant assumption that the unknown closure terms depend only on the instantaneous average variables (and not on any average descriptions of the unresolved flow, such as the turbulent kinetic energy, or on any history effect).

The data generated by the DNS for channel bubbly flows is averaged over planes parallel to the walls, resulting in a database containing the average gas flux, liquid streaming stresses, and surface tension force, along with void fraction, void fraction gradient, gradient of the average vertical liquid velocity, and the distance to the nearest wall, at the horizontal grid point, at all time intervals. We now assume that each of the first three quantities depends uniquely on the latter four, at least in some average sense (since we expect considerably scatter):

$$F_g = f(x), \quad < u'v' >_l = g(x), \quad (f_\sigma)_y = s(x),$$

(2.8)

where

$$x = \left(\frac{\partial < v_l >}{\partial x}, \alpha_g, \frac{\partial \alpha_g}{\partial x}, d_w\right).$$

(2.9)
The functions \( f, g, \) and \( s \) are determined using the DNS database. For the periodic case, since the bubbles are spherical and there is no effect of walls, so there are only two unknown closures \( F_g \) and \( < u'v' >_l \) correlated with three averaged quantities \( \frac{\partial < v >}{\partial x}, \alpha_g \) and \( \frac{\partial \alpha_g}{\partial x} \).

These functional relationships can be predicted by many advanced regression methods [Kuhn and Johnson, 2013], and to model the periodic cases, we choose NN. The multilayer NN is a powerful nonlinear regression technique, typically with a three-layer architecture called input layer, hidden layer and output layer. Each unit in the hidden layer is transformed by a nonlinear function of a linear combination of all the variables in the input layer. Once the hidden units are defined, another linear combination connects all the hidden units to the output units. Take the NN modeling of \( f(x) \) for the \( F_g \) as an example: suppose there are \( m \) input units and \( n \) hidden units, then

\[
h_i(x) = s(a_{0i} + \sum_{j=1}^{m} x_j a_{ji}),
\]

\[
f(x) = b_0 + \sum_{i=1}^{n} b_i h_i(x),
\]

where we use the hyperbolic tangent sigmoid function \( s(u) = 2/(1 + e^{-2u}) - 1 \), as the transfer function. The adjustable coefficients \( a_{0i}, a_{ji}, b_0, b_i \) are found during the training of the NN.

Software packages to train neural networks are widely available and we have used the neural network toolbox in Matlab [MATLAB, 2017] for the periodic case, and Caret package [Kuhn, 2016] in R for the vertical channel cases.

The Matlab toolbox uses a three-layer neural network architecture with feed-forward back-propagation and the Levenberg-Marquardt method to optimize the weight coefficients, which connects the three inputs, ten neurons, and one output for each closure relation. We have experimented with different solution algorithms,
different number of neurons, as well as with more hidden layers, and find that a single hidden layer with ten neurons and the solution algorithm used here give a good balance between accuracy and robustness. The starting values for the weights are chosen to be random numbers near zero. Once the training is done, Matlab returns functions that relate the input variables to the output and here the fitting results in two functions, one for the gas flux and another for the streaming stresses. These functions are then used in a Matlab program to solve equations (2.4) and (2.7).

For the vertical channel case, to reduce the variance between training sessions with different initial values, two additional techniques are combined here: in the first method we create several NN models using different randomly selected starting coefficients, and aggregate all the NN models to generate the averaged NN fit. The procedure, Model Averaging Neural Networks (MANN), has been shown to result in more stable predictions with fewer uncertainties [Perrone and Cooper, 1993, Ripley, 1996, Tumer and Ghosh, 1996]. The other technique is to use resampling and bagging the data during the training of each NN, where we resample the training data with replacement for each NN’s training dataset before aggregating all the models. This has been shown to result in improvements for unstable procedures like NN and decision tree method [Bishop, 1995, Breiman, 1996].

For the wall-bounded vertical channel case, we use the MANN and data resampling techniques, which are available in the Caret package, implemented in R by [Kuhn and Johnson, 2013]. The final NN is averaged by 5 NNs, each with a 3 layer structure: 4 inputs, 12 neurons and 1 output for each unknown closure. All the unknown coefficients for each NN start randomly below 0.1 and the maximum number of iteration for each NN’s training is 250. We have tested the “tuning” parameters such as the range of small starting random numbers, number of neurons, iteration steps, and the number of NNs needed before aggregation, and selected the numbers given here for the best performance. Once the training process is done, Caret package
returns functions that relate the input variables to the outputs and here the fitting results in three functions for the unknown closures. These functions are then used in a R program to solve equations (2.4) and (2.7).

To gather data for the “training” of the NN, we uniformly sample the data from the time interval 0 – 5 for the fully periodic case, even though we have the DNS data running until time 25, the evolution reaches a statistically state at the later stage. For the vertical channel case, we pool all the spatial and temporal data together, and select the frequency of the training data following an exponential distribution based on time, since for the upflow case considered here. The bubbles are initially driven relatively quickly to the wall, but at the late stage the flow evolves very slowly.

Neural networks are, of course, not the only statistical learning technique that can be used, and we have also experimented with linear regressions for the vertical channel case. Unlike MANN, where the functional form of the closure terms are unknown, here we postulate a functional form for the relationship with unknown coefficients and determine the unknown coefficients from the DNS data. We assume that the formula for gas flux is:

\[
F_g = C(-\text{sign}(\frac{d < v > l}{d_x})) \alpha_g^m (\frac{d < v > l}{d_x})^n d(x)^p. \quad (2.12)
\]

The direction of the gas flux is modeled by adding the \(-\text{sign}(\frac{d < v > l}{d_x})\) term, since the sign the of the gas flux is determined by the direction of the lift force. Considering the gas flux to be correlated with \(\alpha_g, \frac{d < v > l}{d_x}\) and \(d(x)\), the distance to the nearest wall, we propose a nonlinear closure with unknown powers. We fit the unknown parameters from the same DNS data used for neural networks’ training and use the bootstrap method to reduce the uncertainty of the training results. We note that we have not included the gradient of \(\alpha_g\), since at locations where \(\frac{d \alpha_g}{d_x} = 0\), the gas flux \(F_g\) is not necessarily zero.
2.4 Feature selection for turbulent quantities

Before the turbulent bubbly modeling is validated, the first challenge is primarily to determine what are the proper closures to model and how to best describe the unresolved state. Bubbly flows in turbulent vertical channels are simulated using a vertical channel between two parallel walls, with periodic boundary conditions in the stream-wise and span-wise direction. The flow is initially turbulent and driven by an imposed pressure gradient with both moving wall and stationary wall boundary conditions. We note that at this point we are not solving model equations for those flows (like the two laminar cases) and once we have decided what variables are preferred, the problem of finding equations for those variables remains.

Unlike the laminar system in the third and fourth chapter, in which closure terms are horizontal bubble flux, streaming stress and average surface tension in a two equation system, we find the horizontal bubble flux might not be a proper closure term in turbulent system to model. Thus, in the fifth chapter, we adopt a new three-equation planar average system, derived from averaging both the x-momentum and y-momentum DNS equation in stream-wise direction, in additional to the equations (2.4) of the average liquid volume fraction. The averaged equation for the vertical liquid velocity \( <v>_l \) is:

\[
\frac{\partial}{\partial t} \alpha_l < v >_l + \frac{\partial}{\partial x} \alpha_l < u >_l < v >_l = \\
- \frac{1}{\rho_l} \frac{dp}{dy} - \frac{1}{\rho_l} \alpha_l \mu_l g_y + \frac{1}{\rho_l} \frac{\partial}{\partial x} \left( \alpha_l \mu_l \frac{\partial < v >_l}{\partial x} \right) - \frac{\partial}{\partial x} \left( \alpha_l < uw >_l \right) + (f_\sigma)_y. \tag{2.13}
\]

The averaged equation for the horizontal liquid velocity \( <u>_l \) is:

\[
\frac{\partial}{\partial t} F_l + \frac{\partial}{\partial x} < u >_l F_l = \\
- \alpha_l \frac{1}{\rho_l} \frac{dp}{dy} >_l + 2 \nu \frac{\partial^2}{\partial x^2} \alpha_l < u >_l - \frac{\partial}{\partial x} \left( \alpha_l < uu >_l \right) + \frac{1}{\rho_l} (f_\sigma)_x. \tag{2.14}
\]
and together with the liquid flux equation:

\[
\frac{\partial \alpha_l}{\partial t} + \frac{\partial F_l}{\partial x} = 0.
\] (2.15)

Thus the relations are ready to learn become:

\[
< \frac{dp}{dy} >_l = f(x), \quad < u'u' >_l = g(x), \quad < u'u' >_l = u(x), \quad (f_\sigma)_y = s(x),
\] (2.16)

First we examine the importance of several average variables (both resolved and unresolved ones describing the unresolved flow), and then we use neural network to correlate the closure terms to all the possible variables, as well as a reduced set of variables. The fitting performance of each cases will be measured using the DNS data.

The importance of each variable is found using recursive feature elimination based on random forest algorithm. Two machine learning packages have been tried based on the R platform. One is implemented in the Caret R package that uses a random forest algorithm at each iterations step and evaluates the model based on Receiver Operating Characteristics (ROC) curve and mean decrease gini (for a general discussion, see [Kuhn and Johnson, 2013]). The variables considered include 14 parameters with both large scale and turbulent scale like the second invariant of the rate of deformation tensor, various variables describing the turbulence, the area concentration and the various area projections. We expect that this list will change as we gain more experience in processing the data and, in particular, that we may need to combine and normalize them in various ways. The other package we have explored is the Boruta R package by [Kursa and Rudnicki, 2017]. The learning algorithm is similar to the Caret package but with an advanced data sampling method, so a uncertainty bound of each parameter’s importance could be estimated as well. Both packages produce nearly the same estimates for the feature selection.
CHAPTER 3

MODELING BUBBLY FLOWS IN FULLY PERIODIC SYSTEM

In this chapter the flow considered consists of several nearly spherical bubbles rising in a periodic domain where the initial vertical velocity and the average bubble density are homogeneous in two directions but non-uniform in one of the horizontal directions. A comprehensive training case is studied to learn the unknown closure models, and then the fitted models are used in the average equations to predict the training cases, as well as other initial conditions to test the generality of the model. Initial attempts on model uncertainty quantification are also done using a Monte Carlo method.

3.1 Model training and testing

Since there are no walls, for nearly spherical bubbles, as we study here, we expect the dynamics of the system to be dominated by the lateral motion of the bubbles from regions of high velocity to regions of low velocity, and the buoyant increase of the vertical velocity of the liquid where the void fraction is high. We have experimented with several different combinations of training and testing cases, but for the results discussed here the training case consists of a uniform distribution of 98 bubbles, resulting in an average void fraction of 9.98%, and an initial velocity profile given by $v(x) = 1.0 \times \cos(\pi x)$. For the parameters used here the slip velocity of the bubbles is about 5 in computational units, so the variations in the liquid velocity are slightly less than half the bubble slip velocity.
Figure 3.1. The bubble distribution for the training case at six times (0.0; 1.25; 2.5; 5.0; 10.0; 20.0). The color shows the magnitude of the vertical velocity, mapping the interval [-0.9, 0.9] to the color interval blue to red.

The first frame shows the initial condition. The bubbles initially concentrated at center, where the velocity is lowest. The large bubble concentration then increases the velocity there, causing the bubbles to spread, eventually making the velocity nearly uniform, as seen in the last frame.
Figure 3.1 shows the bubbles and the average vertical velocity at several times, starting with the initial conditions. The bubbles initially migrate to the region where the velocity is lowest (middle of the domain); then the increased void fraction increases the buoyancy there and thus the velocity. Once the average vertical velocity in the middle is higher than elsewhere in the domain, the bubbles spread out again, eventually resulting in a nearly uniform velocity and a nearly homogeneous distribution of the bubbles. Thus, this DNS data set contains both situations where the bubbles gather together to increase the void fraction locally and situations where the bubbles move to decrease the local void fraction.

To gather data for the “training” of the NN, the DNS results are averaged at time intervals equal to $\delta t = 0.02$, over 256 vertical planes, perpendicular to the $x$ axis. While the simulations are run out to $t = 25$, we only use data for the time interval $0 - 5$. Thus, there are $256 \times 251 = 64,256$ samples, each containing the gas flux, the streaming stresses, the void fraction, the gradient of the void fraction, and the gradient of the average liquid velocity. The data set is divided into three parts by random sampling, one for the actual fitting or training (70% or 44,980 samples), another for validation (15% or 9,638 samples), and one for testing (15% or 9,638 samples). The fitting starts by iteratively adjusting the parameters of the NN to fit the first part of the data. Usually the fitting of the data set improves with the iteration count, but more iterations also result in over-fitting and degrade the ability of the model to predict new data. The validation data is used to detect when this starts to happen and to stop the iterations. Finally, the model is checked by comparing its predictions with the testing part of the data set. We have tried splitting the data set differently and generally find that the fitting is insensitive to how we divide it up.

To examine the quality of the fit, figure 3.2 shows the distribution of the error for both the gas flux (top) and the streaming stresses (bottom). The abscissa is the
Figure 3.2. The distribution of the error for the gas flux (top) and streaming stresses (bottom).
error and the ordinate is the number of points with a given error. The training data is blue, the validation data is green and the test data is red. The vertical black line in the center is zero error and it is clear that most of the points have prediction errors close to zero. This is, of course, particularly true for the training data, but even for the test data the number of points with relatively large errors are few.

If the original data was perfect and the model fitted it exactly, then the model would produce the original data. This is, of course, not the case and to examine how well the model and the data align, in figure 3.3 we plot a scatter plot of the predicted gas fluxes (top) and the streaming stresses (bottom) versus the fluxes and stresses for the part of the data set used for the training in the left row, and in the right row for the part of the data reserved for testing the model (that is, the points not used to construct the neural network, nor determine when to stop the iterations).

The diagonal solid line is the perfect agreement line where the predicted fluxes and stresses are exactly equal to the DNS fluxes and stresses and the dashed line, which has a slightly different slope, is the best fitting line. The correlation coefficient is shown above each frame. For the gas fluxes the solid and the dash lines are nearly parallel and the correlation coefficient is high. The correlation for the streaming stresses is not quite as good, but nevertheless it is still reasonably high. While the correlation coefficient for the test data is slightly lower than for the training data, they are close in both cases.

After using the NN to find $f$ and $g$, we apply the model to predict the evolution of the original data set and in figure 3.4 we show the average velocity and void fraction as found by averaging the DNS data and as predicted by the average model, at six times. Since the flow evolves fast in the beginning and more slowly later, the frames are at non-equal time intervals. The average velocity is shown in the left column and the void fraction in the right one, with the initial conditions in the top row. The initially uniform void fraction quickly increases in the middle of the domain, where
Figure 3.3. The value for the gas fluxes (top) and the streaming stresses (bottom) predicted by the model versus the DNS data. The left column shows the training data and the right column shows the test data.
the velocity is lowest, as the bubbles move down the velocity gradient. The buoyancy there increases the local velocity, eventually producing a velocity slightly above the average, as seen in the fifth frame. This reverses the gas flux, first reducing the void fraction in the middle and eventually producing a more uniform, but unsteady, void fraction distribution. Although the DNS data for the void fractions shows slightly more fluctuations than the model predicts at late stage, overall the model reproduces the averaged DNS results.

To quantify the difference between the model predictions and the averaged DNS data, in figure 3.5 we show an integral comparison between the DNS results and the model results by plotting the root mean square difference between the local void fraction and the liquid velocity and the average value (or the variance), integrated across the domain, versus time. More specifically, those are defined by

\[
< v >_{\text{rms}} = \sqrt{\frac{1}{l} \int (\langle v \rangle (x) - \langle v \rangle_{\text{avg}})^2 dx}, \quad (3.1)
\]

\[
\alpha_{\text{rms}} = \sqrt{\frac{1}{l} \int (\alpha(x) - \alpha_{\text{avg}})^2 dx}, \quad (3.2)
\]

where \(l\) is the period in \(x\) direction.

For our specific setup, the average velocity \(\langle v \rangle_{\text{avg}}\) is, of course, zero. The agreement is reasonably good, as we expect from figure 3.4. Notice that the root mean square difference for both the void fraction and the vertical average liquid velocity does not become zero, for the time examined, and that the model predicts the level of the non-zero root mean square difference, as well as the time scale of the initial change. We do, of course, expect the model to reproduce the original data reasonably well, since the model was derived using precisely this data.
Figure 3.4. The average vertical velocity (left) and void fraction (right) as found by averaging the DNS data and as predicted by the average model, at the six times shown in figure 3.2.
Figure 3.5. The root mean square difference between the local vertical velocity and the average velocity (top) and the root mean square difference between the local void fraction and the average void fraction (bottom), versus time, as found by averaging the DNS training data and as predicted by the average model.
### TABLE 3.1

**THE VARIOUS INITIAL CONDITIONS USED TO TRAIN AND TEST THE MODEL FOR THE CLOSURE TERMS**

<table>
<thead>
<tr>
<th>Case</th>
<th>Initial velocity</th>
<th>Initial void fraction</th>
<th>$MSD(&lt;v&gt;_{\text{rms}})$</th>
<th>$MSD(\alpha_{\text{rms}})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Train</td>
<td>$\cos \pi x$</td>
<td>uniform $\alpha_g =$9.98%</td>
<td>0.02739</td>
<td>0.007075</td>
</tr>
<tr>
<td>Test 1</td>
<td>$\cos \pi x$</td>
<td>uniform $\alpha_g =$4.99%</td>
<td>0.03347</td>
<td>0.009842</td>
</tr>
<tr>
<td>Test 2</td>
<td>$2 \cos \pi x$</td>
<td>uniform $\alpha_g =$9.98%</td>
<td>0.04135</td>
<td>0.017491</td>
</tr>
<tr>
<td>Test 3</td>
<td>$2 \cos \pi x$</td>
<td>uniform $\alpha_g =$4.99%</td>
<td>0.07550</td>
<td>0.007843</td>
</tr>
<tr>
<td>Test 4</td>
<td>$\cos 2\pi x$</td>
<td>uniform $\alpha_g =$9.98%</td>
<td>0.03665</td>
<td>0.010543</td>
</tr>
<tr>
<td>Test 5</td>
<td>$\cos 2\pi x$</td>
<td>uniform $\alpha_g =$4.99%</td>
<td>0.03451</td>
<td>0.007719</td>
</tr>
<tr>
<td>Test 6</td>
<td>$\cos \pi x$</td>
<td>centered $\alpha_g =$4.99%</td>
<td>0.02464</td>
<td>0.016551</td>
</tr>
<tr>
<td>Test 7</td>
<td>$\sin \pi x$</td>
<td>centered $\alpha_g =$4.99%</td>
<td>0.04432</td>
<td>0.010229</td>
</tr>
</tbody>
</table>

3.2 Model validation: applying the model to different initial conditions

To see if the relationship has a more general validity, we have evolved several different initial configurations using the model, with $f$ and $g$ found using the training set described above, and compared the results with DNS of the same initial conditions. The cases are listed in Table I, and in figure 3.6 we show the average velocity and void fraction at six times for case 7, as predicted by the model and found from the DNS results.

The velocity field is the same as in the training case—shifted by half a period by using $\sin(\pi x)$ instead of $\cos(\pi x)$—but the bubbles are concentrated in the middle of the domain where the average void fraction is about 20%. The average void fraction over the whole domain is 4.99%. The evolution is different from the training case in that the bubble distribution is initially moved to the right, to where the velocity is
Figure 3.6. The average vertical velocity (left) and void fraction (right) as found by averaging the DNS training data and as predicted by the average model, at six times for Test 7 in Table 3.1.
lowest. Once the bubbles are there, the increased buoyancy increases the velocity and eventually both the velocity and the void fraction become relatively uniform. The root mean square difference between the local void fraction and the liquid velocity and the average value, integrated across the domain, is shown versus time in figure 3.7 and while the agreement is not quite as good as for the training data (figure 3.6), it is clear that the model still predicts the DNS data reasonably well.

We have examined all the initial conditions listed in Table 3.1 in the same way and find similar results. In figure 3.8 we plot the difference between the root mean square differences, or the variances, as predicted by the model and found from the DNS data, versus time, for all the tests in Table 3.1 (that is, the difference between the dashed and the solid curves in figures 3.7 and 3.8). Again, the agreement is worse than for the training data (shown by the blue solid line), but in all cases the differences between the model predictions and the DNS data are of comparable order of magnitude.

The results are condensed even further in the two rightmost columns in Table 3.1 where the mean square different of the variances, defined by

\[
MSD(< v >_{rms}) = \sqrt{\frac{1}{T} \int ((< v >_{rms})_{DNS} - (< v >_{rms})_{model})^2 dt}, \tag{3.3}
\]

\[
MSD(\alpha_{rms}) = \sqrt{\frac{1}{T} \int ((\alpha_{rms})_{DNS} - (\alpha_{rms})_{model})^2 dt}, \tag{3.4}
\]

are listed, here \( T = 25 \).

We have examined a number of other quantities to evaluate the performance of the model, such as the various correlation coefficients. In many cases we find that those are not particularly useful, since often most of the data points are clustered relatively randomly around the average value and the main contribution to the fit comes from relatively few points far from the average. For the particular setup used
Figure 3.7. The root mean square difference between the local vertical velocity and the average velocity (top) and the root mean square difference between the local void fraction and the average void fraction (bottom), versus time, as found by averaging the DNS training data and as predicted by the average model, for Test 7 in Table 3.1.
Figure 3.8. The absolute value of the difference between the variance predicted by the model and found from the DNS data versus time for all the initial conditions in Table 3.1. The results for the average velocity are shown in the top frame and for the void fraction in the bottom frame. The differences have been normalized by the maximum value of $\langle v \rangle_{rms,DNS}$ and $\alpha_{rms}$ in the DNS results.
here, the largest values of the fluxes and the streaming stresses occur relatively early in the simulations so the early times contribute most to the fitting, and this is the reason that for the results presented here we have used only the data for the first 5 time units. In other simulations we have used the whole set and find similar results. We have also repeated the study presented here by swapping the training case for one of the test cases from Table 3.1 and find that the results are comparable. When we use data from two cases with different setup (such as the current training set and test case 6) for the training we find that while the training error does not decrease significantly, the robustness of the model increases in the sense that the errors for all the test cases are comparable. This is probably not surprising. In general we find that the closure for the gas flux, $F_g$, and how it is modeled, is critical for the correct prediction of the evolution of the flow, including both its structure at any given time and the rate at which it changes. The streaming stresses, on the other hand, play a much smaller role, at least for the parameter values examined here, and we find, for example, that taking them to be zero results in relatively minor increase in the difference between the DNS and the model results. The closure relationships found here are, of course, only valid for the particular set of governing parameters selected here. If we make the bubbles larger or smaller the Eötvös ($Eo$) number changes and if it becomes sufficiently high the bubbles are no longer nearly spherical and we would expect the closure relationships to change. However, if the bubbles remain nearly spherical, the dynamics does not depend on $Eo$ and we expect reasonably good agreement. We could, of course, expand the dataset to include the governing parameters, in which case we expect to be able to use the model for a larger range of situations.
3.3 Model uncertainty quantification

In earlier chapters statistical learning is used to develop relationships between closure terms in an averaged model and the large scale averaged quantities evolved by the model equations. The remaining work is to measure the the accuracy of this method considering the uncertainties in the data, thus uncertainty quantification (UQ) of the model will be discussed this here.

To quantify the uncertainty of the training procedure, we conduct the Monte Carlo sampling on the training process for several times, generating relatively large samples of learned closures. Then we implement these trained models into the averaged equation and record the quantities of interest (QOIs) for each model as time evolves. These QOIs samples are used to quantify the uncertain of the model and calculate the corresponding error bond for the training.
In figure 3.9 we can see that at each time step, the predicted value of the QOIs (dash lines) has the mean value close to that of the DNS data (solid line). Even though there are some values with relative larger fluctuations, most of the predicted values are clustering around the DNS value. Similarly, to quantify the uncertainty of the model testing procedure, we still use the same closure model samples learned from the training data, and apply each of them to different situations during the test, and record the QOIs as well for new situations.

The preliminary results have shown that while the results show some scatter, the mean value of QOIs closely follows the DNS prediction, as shown by figure 3.10.

When we applied the trained models to different test cases, the data used to “train” the NN ideally needs to contain the situations (patterns) that the systems that we want to predict are likely to encounter. Figure 3.11 and figure 3.12 show a simpler test case with $\alpha_g = 0.49$, which is only half of void fraction of the training
Figure 3.11. Plot of the predicted $\alpha_{rms}$ with different training models and the DNS value of $\alpha_{rms}$ in a simpler test case.

Figure 3.12. Plot of the averaged predicted $\alpha_{rms}$ with different training models and the DNS value of $\alpha_{rms}$ in a simpler test case.
Figure 3.13. Plot of the predicted $\alpha_{rms}$ with different training models and the DNS value of $\alpha_{rms}$ in a more complex test case.

Figure 3.14. Plot of the averaged predicted $\alpha_{rms}$ with different training models and the DNS value of $\alpha_{rms}$ in a more complex test case.
case, and in this case the model predictions are relatively good and the mean value of the QOIs closely follows that of the DNS data, and the variance of the model is relatively small at each time step.

However, as the test cases become complex, in certain region of the parameter space, the training case may be short on data. Even though the mean value of the predicted quantities is close to the DNS data, the prediction variance becomes larger, just as figure 3.13 and figure 3.14 show. For more complex test case with $\alpha_g = 0.98$ and the maximum shear rate twice as large as that of the training case, the predictions can be somehow overshot or undershot at early time because of short on data in parameter space with high shear rate and high void fraction.

3.4 Conclusion

In this chapter, we started with a relatively simple system to set up the frameworks for using machine leaning to close reduced order models and to design different DNS test data to demonstrate the validation of the model.

First of all the model is homogeneous in two directions so the averaged equations have only one spatial coordinate. Secondly, it is periodic in all directions and there are no walls, and thirdly, no average descriptions of unresolved quantities appear to be necessary (which might be governed by their own evolution equations with unknown closure terms). Furthermore the gas flux appears to a function of the local state only and no evolution equation for the bubble velocity needs to be solved. Most multiphase flows are considerably more complex than the system considered here, but we believe that there is nothing that intrinsically limits using data mining for the closure terms to simple systems only.

We have examined the use of neural networks to fit DNS data to develop closure relations for the average two-fluid equations for a simple fully periodic bubble system. The neural network is trained on one DNS data set and then applied to other flows
where the initial velocity and void fraction are different, but for which we also have DNS results to compare with. Overall, the average equations with the neural network closure reproduce the main aspects of the DNS results, including the generally rapid change initially as well as the level of unsteadiness remaining after the initial adjustment.

Indeed, it is probably fair to say that the level of agreement is somewhat unexpected given the small size of the training data and the relatively high level of fluctuations observed in the DNS results. The approach taken here should allow us to quantify the uncertainty of the model and how it depends on the size of the training data [Rajabi and Kavianpour, 2012]. However, this quantification, as well as propagating this and other uncertainties [Hastie et al., 2001], such as in the initial conditions, to the final predictions, remains to be done.

We also note that there are several versions of neural networks and related approaches [Bishop, 2006] and we have made no effort to find the best one. Perhaps the biggest drawback of the neural network is that there is little physics in the fitting. This is, presumably, both a strength and a weakness. We do not need to know much about the physics to obtain the closure modeling, but conversely a knowledge of the physics is of little help, at least for the approach taken here.
CHAPTER 4

MODELING BUBBLY FLOWS IN LAMINAR VERTICAL CHANNELS

In this chapter, bubbly up-flow in a periodic vertical channel is used to generate closure relationships for the two-fluid model for the average flow. Nearly spherical bubbles, initially placed in a fully developed parabolic flow, are driven relatively quickly to the walls, where they increase drag and slowly reduce the flow rate. Once the flow rate has been decreased enough, some of the bubbles move back into the channel interior and the void fraction there approaches the value needed to balance the weight of the mixture and the imposed pressure gradient. A database is generated by averaging the DNS results over planes parallel to the walls, and a Model Averaging Neural Network (MANN) is used to find the relationships between unknown closure terms in a simple model equations for the average flow and the resolved variables. The closure relations are then tested, by following the evolution of different initial conditions. We also include results using linear regression for the closures.

4.1 Model training and testing

The results shown in figure 4.1 provide the training data for our model, which shows the bubble distribution and the velocity contour at the mid plane in the span-wise direction at six different times. The first frame is at time zero where the flow is parabolic and the bubbles are spread nearly homogeneously across the channel. In the next frame, most of the bubbles have moved toward the wall. There is a clear layer of bubbles at both walls, and only a couple of bubbles in the middle. The bubble motion is fairly unsteady and the wall-layer is often broken up by the motion
Figure 4.1. The bubble distribution for the training case at six times (0.0; 10.0; 20.0; 40.0; 80.0; 140.0). The color shows the magnitude of the vertical velocity at the mid-plane in the z-direction, mapping the interval [0.0, 2.0] to the color interval blue to red. The first frame (top left) shows the initial condition.
of the bubbles just outside of it. This development continues in the third frame, where the middle of the channel is mostly free of bubbles. In the fourth frame, all the bubbles are near the walls, and in frame five, the bubbles stay close to the wall, but the average liquid velocity is lower. In the sixth frame, at a much later time, some of the bubbles have moved back into the channel interior and the void fraction there approaches the value needed to balance the weight of the mixture and the imposed pressure gradient. Before we plug in the models for the closure terms into the averaged equations, we need a reliable training procedure for the neural networks. We collect various quantities averaged over planes parallel to the walls, together with the unknown closure terms, at different times and use neural networks for the fittings. Here we assume that the unknown closure terms in equations (2.4) and (2.7) depend only on the averaged quantities and not on any average description of the unresolved field. Obviously there cannot be any dependency on $<v>_l$ directly, so to the lowest order we assume a dependency on the velocity gradient. The closure terms can, however, depend on the void fraction and we include the possibility that there is also a dependency on the gradient of $\alpha_g$. We have done a test of the model variable selection, and in [Ma et al., 2015] these three variables were found to be enough. For wall bounded flow we must also allow for a possible dependency on the distance to the wall $d_w$. Figure 4.2 shows the quality of the fitting.

In the left column we show a histogram of the training error distribution for the gas fluxes, streaming stress and surface tension force. Most of the training errors are clustered around zero, and the number of instance falls off rapidly as the error becomes larger. The distribution is close to Gaussian, though there is a slight skewness. In the right column we show a scatter plot of the predicted average gas fluxes versus the average fluxes from the DNS for the test data. Although there is some spread, the points are mostly clustered around the forty five degree line.
Figure 4.2. The training error histograms (left column) and the regression plots (right column) for the three closure terms: $F_g$, $<u'u'>$, and $f_{\sigma}$. 
The output from the Caret package is a function which maps the correlated variables to the unknown closure, and we use these functions for each closure term in an R code to solve equations (2.4) and (2.7). The predictions of the model are shown in figure 4.3 where we plot the average liquid velocity at five times in the left column and the void fraction at the same times in the right column, along with the averaged DNS results and from the model where the closure terms are found by linear regression. The results again show that when nearly spherical bubbles are injected into parabolic flow the evolution toward steady state is highly non-monotonic. First, all the bubbles migrate towards the walls, leaving the centre region nearly free of bubbles. Then the presence of the bubbles near the wall increases the friction there and reduces the flow rate. As the flow rate is reduced sufficiently some of the bubbles migrate back into the core region until the mixture there is in hydrostatic equilibrium. Thus, the initially parabolic velocity decreases rapidly in the middle of the channel and is nearly uniform across almost all of the channel at the last time shown, going to nearly zero only very near the walls. The void fraction profile is more complex but a careful inspection shows that the bubbles rapidly accumulate near the walls, with the void fraction going to zero in the middle of the channel and then returning to a profile consisting of nearly uniform value across most of the channel with peaks near the walls in a layer of thickness of about one bubble diameter. The initial migration of the bubbles to the wall takes place relatively fast, but the slowing down of the flow and the migration of the bubbles back into the core is a much slower process. Here we do not allow the bubbles to coalesce, but if they could then the migration to the wall might promote the formation of either larger bubbles that would move away from the wall relatively quickly or possibly a gas film at the wall.

The linear regression is more sensitive to the data sampling techniques and data size than the MANN. Here a bootstrapping method is used for selecting the data with replacement for 2000 times (we gradually increase the data sample size from
Figure 4.3. A comparison of the prediction of the model with averaged DNS data. The average liquid velocity is shown on the left, at several times, and the average void fraction on the right.
TABLE 4.1

THE ESTIMATED REGRESSION COEFFICIENTS AND CORRESPONDING STANDARD DEVIATIONS WITH BOOTSTRAP

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Mean value</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>2.84e-2</td>
<td>2.24e-3</td>
</tr>
<tr>
<td>m</td>
<td>6.54e-1</td>
<td>6.88e-2</td>
</tr>
<tr>
<td>n</td>
<td>7.88e-1</td>
<td>6.68e-2</td>
</tr>
<tr>
<td>p</td>
<td>3.77</td>
<td>5.57e-1</td>
</tr>
</tbody>
</table>

500, and end at 2000), generating 2000 sub-dataset. In each subset we do a linear regression and then take the mean value of the unknown coefficients and estimate its standard deviation, in order to reduce the uncertainty and get more reliable results. Using bootstrap we can also estimate the standard deviation for each coefficient, as given in Table 4.1

In addition to directly checking the average void fraction and liquid velocity, we have also examined the unsteady evolution of the flow as shown in figure 4.4 and 4.5, where we plot the average wall shear (top) and the average flow rate (bottom) as obtained from DNS data and from the model, where the liquid flow rate $Q$ and average wall shear rate $\gamma$ are defined as:

$$Q = \int_{0}^{H} < v >_{l} \, dx, \quad \gamma = \frac{d < v >_{l}}{dx}|_{x=0}$$

Initially the shear stress is in balance with the steady state flow of the liquid but as bubbles accumulate near the walls, the wall shear increases and the flow starts to slow down. The wall shear quickly reaches maximum, when most of the bubbles are at the wall, and then drops slowly as the flow rate continues to slow down.
Figure 4.4. Averaged wall shear versus time, for the simulation in figure 4.3.

Figure 4.5. Averaged flow rate versus time, for the simulation in figure 4.3.
4.2 Validation of the model: applications to different initial conditions

Ideally the relationship derived in the last section by MANN is sufficiently general so that it can be used for flows that are different from the “training” case. To examine how well it does, while still remaining within the rather restrictive setup in which it was developed, we have examined a few different conditions. Those include: up flow cases with different shear rate; more complex initial velocity shaped as $\sin$ function; down flow cases with different shear rates; and a vertical Couette flow.

In figure 4.6 we show a comparison of the model predictions and averaged DNS data for downflow, at five times, using the closure relationships derived for the upflow presented earlier. The average liquid velocity is shown in the left column and the void fraction at the same times in the right column, along with the averaged DNS results. The changes in the flow are far less dramatic than for the upflow. The bubbles move slightly closer to the channel centre and increase the buoyancy there, flattening the velocity profile, resulting in a nearly uniformly void fraction in the middle of channel and well-defined bubble free layers near the walls.

Similar to the upflow case, figure 4.7 and figure 4.8 respectively shows the comparisons of wall shear rate and liquid flow rate between DNS data and model predictions, for the downflow case. Overall the agreement between the model and the DNS is good and the minor differences observed are mainly during the early times.

In general, if we train and test the model on the same case, we would expect a better prediction performance than testing the learned model on different cases. However, it is not always the truth since we also need to consider the complexity of physics. From figures 4.7 and 4.8, we can see that even though this is the testing case, the closure results in predictions that are even better than for the original training case.

The agreement between the model predictions and the averaged DNS data for other conditions, using the same closure relations, are similar. To summarize the
Figure 4.6. A comparison of model predictions and averaged DNS results for down flow.
Figure 4.7. Average wall shear versus time for the simulation in figure 4.6.

Figure 4.8. Average flow rate versus time for the simulation in figure 4.6.
Figure 4.9. The difference between the liquid flow rate predicted by the model and found from the DNS data versus time for all the initial conditions in Table 4.2. The differences have been normalized by the maximum value of liquid flow rate in the DNS results.

Figure 4.10. The difference between the wall shear rate predicted by the model and found from the DNS data versus time for all the initial conditions in Table 4.2. The differences have been normalized by the maximum value of the wall shear rate in the DNS results.
TABLE 4.2

THE VARIOUS INITIAL CONDITIONS USED TO TRAIN AND TEST
THE MODEL FOR THE CLOSURE TERMS

<table>
<thead>
<tr>
<th>Case</th>
<th>velocity</th>
<th>Initial void fraction</th>
<th>$MSD_1$</th>
<th>$MSD_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Train</td>
<td>$2(-x^2 + 2x)$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.05661</td>
<td>0.002536</td>
</tr>
<tr>
<td>Test 1</td>
<td>$3(-x^2 + 2x)$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.08361</td>
<td>0.006262</td>
</tr>
<tr>
<td>Test 2</td>
<td>$2(x^2 - 2x)$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.01632</td>
<td>0.001637</td>
</tr>
<tr>
<td>Test 3</td>
<td>$3(x^2 - 2x)$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.03955</td>
<td>0.002374</td>
</tr>
<tr>
<td>Test 4</td>
<td>$\sin \pi x$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.04801</td>
<td>0.006202</td>
</tr>
<tr>
<td>Test 5</td>
<td>$-x + 1$</td>
<td>uniform $\alpha_g = 4.99%$</td>
<td>0.07569</td>
<td>0.004565</td>
</tr>
</tbody>
</table>

results, we show in figure 4.9 and figure 4.10 the difference between the model and the DNS data versus time, for six cases, listed in Table 4.2. The results are condensed even further in the two rightmost columns in Table 4.2 where the mean square different of the error, defined by

$$MSD_1 = \sqrt{\frac{1}{T} \int (\gamma_{DNS} - \gamma_{model})^2 dt}, \quad (4.2)$$

$$MSD_2 = \sqrt{\frac{1}{T} \int (Q_{DNS} - Q_{model})^2 dt}, \quad (4.3)$$

In all cases the differences between the model predictions and the DNS data are of comparable order of magnitude, unlike the situation in periodic cases, where the agreement is generally worse than for the training data. For wall bounded bubbly flow, the training case itself is more complex in physics than some of the testing cases, like the downflow cases.
4.3 Closure terms analysis

The results of the fitting, using the neural network, are transferred to the numerical implementation of the model as functions that can be treated as a “black box”. A visual inspection does, however, help us evaluate the quality of the fit and understand what physical processes are captured. In figure 4.11 and 4.12, we show how the gas fluxes, the streaming stresses and surface tension force depend on the average liquid shear rate. In the figure 4.11 we set the void fraction equal to \( \alpha_g = 0.1 \) and show the relationships as the distance to the wall gradually increases. In the figure 4.12 the distance to the wall is set to two bubble diameters and we show the flux for a few different void fractions. The wall distance function is linear and reaches its maximum value 1 at the centre of the domain. We have also experienced with other types of wall distance function and did not find much difference since the NN automatically adjusts the power of the wall distance function. For zero velocity gradient the gas fluxes are zero and for gradient near zero the gas fluxes are a decreasing function of the liquid shear rate, as we would expect for nearly spherical bubbles. The flux is lowest for bubbles close to the wall and the effects of the wall become smaller as \( d_w \) increases. Eventually we would expect the wall to have no effect and the dashed line in figure 4.11 is a fit from simulations with no walls. Obviously the current results away from the walls agree well for low shear rates. As the shear rate is increased, however, the flux reaches a maximum and then decreases. This can, at least in principle, be due to two effects: The increased shear deforms the bubbles more and thus the lift changes sign, or this can be a result of the highest shear being found close to the walls, where the flux is reduced due to wall effects and not deformability. This is probably the latter, as discussed below.

The fit for the streaming stress shows a similar trend. For zero shear the stress is zero and for low shear rate it is a decreasing function of the liquid shear rate. It is lowest close to the wall and its dependence on the distance to the wall is reduced.
Figure 4.11. The closure term $F_g$ as functions of the liquid shear rate with different distances to the wall at fix value of void fraction $\alpha_g = 0.1$.

as we move further away. As the top frame in figure 4.13 shows, the slope of the streaming stress is converging to a constant value in the low shear rate region, as the distance to the wall increases, and approaches the slope fitted by the periodic case without walls, shown by the dash line.

The bottom frame of Figure 4.13 shows the average surface tension term versus the fluid shear. The distance to the wall is fixed at two bubble diameter. As the void fraction increases, more bubbles are near the wall, so the surface tension force increases. Looking at the fluxes directly can give us insights into the closure relationships and allow us to examine that they are aligned with our intuition. Such an inspection can help us identify problems. In our case, for example, the gas fluxes go to zero for high shear rate for any distance to the wall. While it is true that high shear rates deform the bubbles and reduce lift and thus gas flux, the reason is much more likely to be that we do not have any data points for high shear away from the walls. The similar behavior for the streaming stress is likely to be for similar reasons.
Figure 4.12. The closure term $F_g$ as functions of the liquid shear rate with different void fractions at fixed distance to the wall at two bubble diameters.

The gas flux and other closures have also been examined with the linear regression and they are generally in good agreement with the values predicted by the MANN, as shown in figure 4.14, where the gas fluxes are plotted versus the shear rate in the liquid, for two values of the void fraction and a distance to the wall equal to two bubble diameters, as obtained by both approaches.

4.4 Conclusion

Here we extend the studies from chapter 3 and examine how DNS results can be used to provide closure relations for vertical channel bubbly flow modeling. We have done this in the context of a fairly simple setup, following the transient evolution of bubbly flow in a vertical channel. The bubbles are all of the same size, the initial liquid velocity is taken to be laminar and parabolic, and the Reynolds number is sufficiently low so that velocity disturbances are likely to be only due to the bubble motion. We use a model averaging neural network that is trained on one DNS data
Figure 4.13. The closure term \( <u'v'>_t \) as functions of the liquid shear rate with different distances to the wall at fix value of void fraction \( \alpha_g = 0.1 \) (top frame), and the closure term \( f_\sigma \) with different void fractions at fixed distance to the wall at two bubble diameters (bottom frame).
Figure 4.14. Comparisons of fitted closure term $F_g$ with MANN model (solid line) and linear regression model (dash line) at $\alpha_g = 0.1$ (red line) and $\alpha_g = 0.2$ (black line).

set and then applied to other situations where the initial velocity, void fraction and boundary conditions are different in the channel, but for which we also have DNS results to compare with. Overall, the average equations with the neural network closure reproduce the main aspects of the DNS results, including the generally rapid change initially, unsteadiness remaining after the initial adjustment and the final steadiness state.

We have also found that the closure terms by postulating a relationship with unknown coefficients that are found using linear regression. Both approaches give comparable results, but given the slightly better accuracy and their generality, we believe that the neural networks are the preferred approach for more complex flows.

We emphasize that the system considered here as well as the two-equation model are relatively simple. Specifically, no average descriptions of unresolved quantities appear to be necessary (which might be governed by their own evolution equations with unknown closure terms, like the turbulent kinetic energy). This part will be
explore in the fifth chapter. Furthermore, the gas flux appears to be a function of
the local state and no evolution equation for the bubble velocity needs to be solved.
We have also examined a model where a new equation governing the evolution of
gas flux term is added, and the averaged horizontal pressure gradient appears as
a new closure terms instead of gas flux term. The three-equation model does not
dramatically increase the prediction accuracy for the current parameter range. We
close by nothing that while most multiphase flows are considerably more complex
than the system considered here, we believe that there is nothing that intrinsically
limits using statistical learning for the closure terms to simple wall-bounded systems
only.
CHAPTER 5

MODELING BUBBLY FLOWS IN TURBULENT VERTICAL CHANNELS

5.1 Introduction

DNS is now possible for fairly large turbulent multiphase systems with over 500 bubbles and a shear Reynolds number of several hundred. In this chapter, attempts are made to extend the statistical learning to complex turbulent multiphase flow modeling. Compared with modeling of laminar systems, there are several differences: firstly, the averaged equations used in laminar flows may not be the best choice when the flow becomes turbulent. For the laminar cases we tried both the 3-equation system and the 2-equation system described in chapter 2, but no obvious differences were observed. Secondly, the fundamental assumption for the laminar case is that the closure terms can be correlated with the averaged scale quantities. This is not always true for turbulent bubbly flows. In RANS models, additional variables representing the state of the unresolved turbulent scales are needed as key dependent variables for the unknown closure terms.

In this chapter, we first examine bubbly flows without topology changes. The unsteady DNS results of a pressure-driven Poiseuille type bubbly flow will be shown, to give the reader a general view of the data. Before we validate the turbulent model, the most critical question is: what are the target unknown closures and which physical quantities are best for the modeling. Based on the DNS data, we use random forest method for selection selection, where we look for the most important variables to model the closures. After this step, we correlate the selected features to model the unknown closures and again use the DNS dataset for a priori test.
We continue the study with the identification of wall and interior-regions for bubbly flow using DNS data, aiming to explore the feasibility of modeling turbulent bubbly flows in separate zones, as well as methods to make a more comprehensive training dataset by combining cases for different parameters. Finally, similar processes will be applied to turbulent bubbly flows with topology changes.

5.2 Turbulent bubbly flows

For turbulence flow with nearly spherical bubbles, lift forces drive the small bubbles to the wall, forming a bubble-rich wall-layer, while the larger deformable bubbles will mostly stay in the channel interior. The removal of nearly spherical bubbles from the channel interior continues until the two-phase mixture is in hydrostatic equilibrium. The same evolution has been observed in earlier DNS study of laminar and turbulent bubbly up-flows, see [Lu and Tryggvason, 2013].

5.2.1 The structure of turbulent bubbly channel flows

The first challenge of turbulent bubbly modeling is to determine how to best describe the unresolved state. We first work on results for a Poiseuille type flow at a friction Reynolds number of 250. There are 72 bubbles with different sizes, consisting of 60 small ones with a diameter at 0.22 and $Eo = 0.945$, 10 medium ones at a diameter of 0.35 and $Eo = 2.393$, and 2 large ones at a diameter of 0.44 and $Eo = 3.781$, which makes the total void fraction 6.57%. The simulation is done using a vertical channel between two parallel walls, with a width in wall-normal direction of 2, and two periodic boundary conditions in the stream-wise and span-wise directions. The flow is initially turbulent and driven by an imposed pressure gradient and the bubbles are uniformly distributed across the domain.

Figure 5.1 shows the bubble distributions at time 10, when the bubbles are at an early stage, and two subsequent times, 40 and 110. The top three frames show
the bubble interfaces together with the vorticity iso-surface in the stream-wise direction, and bottom three frames also show the contour plot of vertical liquid velocity magnitude at the mid-plane in the span-wise (z) direction.

At the earliest time we see that the vorticity distribution is as we expect for a single phase flow: a peak close to the wall corresponding to hairpin vorticies and then a maximum right at the wall corresponding to the wall-bound vorticity needed to bring the velocity to zero. When the bubbles move toward the wall this changes as in the second and third column of figure 5.1 and we see a significant increase in the vorticity near the wall. It is also clear that at later stage the small bubbles form layers at the walls but the larger ones remain in the middle of the channel. This phenomenon is similar to what we observed in the laminar cases.

In figure 5.2, both the liquid flow rate (top frame) and liquid shear rate (bottom frame) at the wall, respectively, are plotted versus time. The initial conditions are set up such that wall-shear balanced the weight and the pressure gradient, but as the bubbles move to the wall, they increase the wall-shear and the flow must therefore decelerate, as is seen in the liquid flow rate (top frame in figure 5.2). The liquid flow rate is currently decreasing while the liquid shear rate at the wall does not seem to decrease yet, indicating that the system still needs longer time to reach the steady state. Indeed, plots of the flow rate of the liquid and the wall-shear stress versus time show that the system is far away from the steady state where the wall-shear balances the weight of the mixture plus the pressure gradient. Eventually the wall shear rate will start to decrease again and asymptotically approach the steady state value, as shown by the dash line in the wall shear rate (bottom frame in figure 5.2).

In figure 5.3, a few quantities averaged over planes parallel to the walls are plotted, versus the wall-normal horizontal coordinate at four times (10, 60, 100 and 161, all in computational units). The average quantities include the vertical liquid velocity, the bubble void fraction, the turbulent kinetic energy, together with potential closure
Figure 5.1. The evolution of turbulent flow stream-wise vorticity (top frame) and liquid velocity (bottom frame) containing bubbles of several different sizes at three times. The stream-wise vorticity is visualized by iso-surface at magnitude 7 and -7. The liquid velocity contour is shown with magnitude between 0 and 1.
Figure 5.2. The evolution of the liquid flow rate (top frame) and liquid shear rate at the wall (bottom frame). The dash line shows the steady state value of the liquid shear rate at the wall.
terms like gas flux, Reynolds stress terms $< u'v' >$ and $< uu' >$. It is clear that
the average liquid velocity (bottom right frame) has not changed much so far. This
is as expected since the small bubbles must first move to the wall to form a layer
before the presence of the layer starts to influence the velocity. While the average
velocity has not changed much, the void fraction (top left frame) has. Initially, the
bubbles are relatively uniformly distributed but as they start to move upward the
small bubbles start to migrate toward the wall. This leads to an increase in the void
fraction there and at the latest time the distribution has almost reached the steady
state value. This suggest that care must be exercised when interpreting short time
results for turbulent bubbly flows since the results may appear to be at steady state
whereas they actually are still evolving but on a relatively long timescale. As the flow
evolves further, however, we expect the presence of the bubbles at the wall to reduce
the flow rate. Experience with bubbles in turbulent up-flow at smaller Reynolds
numbers and in smaller laminar systems suggest that this will take significant time.
As the void fraction distribution in the top left frame shows most clearly, the flow is
evolving and given the steady state results for smaller systems and lower Reynolds
numbers we expect its structure to continue to change.

The modest modification of the flow due to the presence of the bubbles at the early
times is also seen in the bottom left frame in figure 5.3, where one of the turbulent
Reynolds stress, $< u'v' >$, is plotted versus the horizontal coordinate. At steady
state, $< u'v' >$ should go to zero in the middle of the channel, if the evolution is the
same as we have seen for smaller systems. The average profile has not changed much
at time 10, and shows the linear shape expected for a single-phase flow.

Plots of the turbulent kinetic energy (second row, first column) and $< uu' >$
(second row, second column) show a slight decrease as the bubbles start to modify
the flow, as in the middle of the channel and in the wall-layer.
Figure 5.3. Evolution of averaged quantities versus wall-normal location of $\alpha_g$, $F_g$, $k$ (turbulent kinetic energy), $\langle u'u' \rangle$, $\langle u'v' \rangle$, $\langle v \rangle$. 
Figure 5.4. Evolution of averaged quantities versus wall-normal location of \( \omega_x \) (vorticity in wall-normal direction), \( \omega_y \) (vorticity in stream-wise direction), and \( \epsilon \) (turbulent dissipation rate).
Additional plots of other averaged quantities are shown in figure 5.4, including the vorticity distribution in the stream-wise and wall-normal direction, as well as the turbulent dissipation rate. As the bubbles start to move and shed vortex, it is clear that the vorticity in the center of the channel increases slightly and that the vorticity structure near the wall starts to change as well. This can also be seen in the figure 5.1. The dissipation rate (bottom frame of figure 5.4) increases both near the walls and in the middle of the channel. This could be attributed to the increase of liquid shear rate at the wall when nearly spherical bubbles start to gather close to the wall, as well as the bubble induced vortex shedding inside the channel interior.

5.2.2 Turbulent feature selection

There are plenty of choices to select the averaged quantities to model the unknown closure terms. Through feature selection, it is possible to determine an optimum reduced set of averaged quantities most closely related to the unknown closures. The reduced set of variables should be sufficient for the closure modeling without sacrificing the predictive accuracy. Once the most critical variables are selected, corresponding governing equations can be generated to follow how these variables evolve. Thus the complicity of the turbulent modeling is reduced.

The feature selection is based on the Recursive Feature Elimination (RFE) algorithm. Initially, all variables are used for the fitting to get the lower bound of fitting error. Then a fixed number reduced set of variables are used in each random tree of the random forest together with the shuffling of the training data. The algorithm then averages the predictions in candidate pools consisting of the possible variables used for the prediction, and votes for the most important variable during each trial. This process is continued with fewer and fewer variables in the candidate pool, and finally we end up with only one variable. During these iterations, the importance of each variable is recorded and finally reported as well. This algorithm is already
Figure 5.5. The root-mean square error (RMSE) (left frame) and the correlation coefficient (right frame) versus the number of variables included.

implemented in the Caret package on R platform using a random forest algorithm at each iteration and evaluates the model performance based on the Receiver Operating Characteristics (ROC) curve and mean decrease gini index. The standard definitions of these statistical quantities will be covered in later sections.

The variables considered so far are the averaged variables used in the simple model presented in the Appendix, including the local liquid shear rate, local void fraction and its derivative, the wall distance function, the second invariant of the rate of deformation tensor $Q$, various variables describing the turbulence such as the turbulent kinetic energy and its derivative, dissipation rate, and the various area concentrations that describe the statistical details of the interface. Recently, several authors [Wu, 2016], [Wang, 2016], [Xiao, 2016] have explored different non-dimensional variables together with invariants as the model inputs. Here we mostly choose the scaler invariant quantities together with their derivatives as the model inputs. We expect that this list will change as we gain more experience in processing the data and, in particular, that we may need to combine and normalize them in certain ways.
Results from the recursive feature selection are shown in the next two figures for the average lateral gas flux. Figure 5.5 shows the root-mean square error (RMSE) (left frame) and the correlation coefficient (right frame) versus the number of variables included. The error decreases and the correlation coefficient increases rapidly with the first six variables. However, after then there are only minor changes, and the learning curve becomes nearly flat.

Figure 5.6 shows the mean decrease gini index for each variable, which is used here to rank the potential variables in order of their importance. The mean decrease gini is shown as a scaled bar-plot with a maximum value of 100, measuring how each variable contributes to the homogeneity of the nodes and leaves in the resulting random forest by [Kuhn and Johnson, 2013]. As expected, the mean shear rate is the most important one, followed by the second invariance of the deformation tensor. This is because the horizontal lift force depends strongly on the liquid shear rate when the bubbles are nearly spherical. This is similar to our previously presented laminar channel flow case.
The learned result of the most important variable is usually very robust. Though there may be some randomness in the rank of the other parameters’ importance, the top 6 variables are relatively stable, based on our numerous training practices.

5.2.3 A priori test for closure terms

The terms “a priori” is to denote the foundations upon which a proposition is known as explained. The behavior of the various models can be extracted by the a priori test, in which a velocity field produced by direct simulation of the N-S equations is used to compute exact unresolved scale quantities and the modeled quantities at many grid points. The exact and modeled values are then compared [Piomelli and Ferziger, 1988]. In our framework, the input data for the model is taken from a DNS simulation, and the results produced by the model, namely the predicted closure terms are compared with those obtained from the DNS data of each unknown closure terms, as the knowable information for the training, validation and testing.

After the feature selection, the next step is to correlate the unknown closures to the selected variables again and use the DNS data for a priori test. We have tried to fit using all the variables and using a reduced set of only the top 6 ranked variables. The number of the reduce set variable is based on the essential dimension of the specific case, as already explained when we discussed the figure 5.5.

To assess how well the gas fluxes are predicted by the most important variables that we have selected, a neural network is used to correlate the gas flux and the selected variables. The reason we use the neural network instead of random forest regression is that the NN can generate a continuous and relatively general closure with a functional form suitable for analysis, which allow us to use 2D or 3D plots to examine the results after freezing several parameter dimensions. This preliminary checking method has been discussed in chapter 4, closure terms analysis.
Figure 5.7. The model prediction versus the DNS data for the full (left) and the reduced (right) dataset. The training data is on the top and the test data on the bottom.
Figure 5.7 shows the gas flux predicted by the model versus the DNS data for both the training and the test data. In the top two frames we use the training data set but in the bottom two frames we use the test data set to explore how well the top six variables in Figure 5.7 describe the flux. Here we use 80% of the data for training and 10% of the data for testing, which are randomly divided based on the whole DNS data. Though the reduced dataset suffers a little bit in performance compared with the full dataset, all of the fitting have a very high correlation level.

5.2.4 Classification of the wall and interior regions

For bubbly flows without topology changes, the bubble drifting mechanism is quite different in the interior-region far away from the wall, where the bubbles do not sense the wall and the wall-distance function becomes unimportant for the closure terms, and for the bubbly wall-layer, which is rich with bubbles due to the strong liquid shear rate near the wall and the added pressure force. Therefore it is natural to model the system separately in each region.

In this section, attempts to model the wall-layer and the interior-region separately will be discussed. First, we check how well the data can automatically support this idea by using key variables as features to classify the data into a interior-region and a wall-layer. Secondly, we have examined whether the same work-flow, using feature selection, followed by NN fitting for a priori test still works well in the separate zones respectively. Generally we expect that the importance of each variable will differ greatly for the different region.

Theoretically, the thickness of the wall-layer is determined by the added pressure and wall shear rate, as can be seen in literature [Lu and Tryggvason, 2013]. Here, for simplification, we have examined several bubble wall-layer thickness, and finally chosen the thickness equal to the smallest bubble diameter. By marking the data inside the wall bubbly layers with a binary feature 1, while the rest of the dataset is
identified by 0, the assumption becomes a binary classification problem. If the data marked with 0 are easily classified as different from the data marked with 1, using properly selected features, that are different in the different zones, then the DNS data indirectly supports the idea of making the model desperately in different zones.

Here we have compared several classification method using the classification package in Matlab, including random forest, support vector machine (SVM) and neural network (NN). Each classification method has its pros and cons. However, the performances of the different classification methods on this dataset are similar. One reason is that the key variables are selected properly and this makes the classification process much easier. Three potential closure terms, the gas flux $F_g$, the streaming stress $< u' v' >$, and the averaged surface tension force $f_\sigma$, which have been previously used as the target closure terms are used as the input variables for NN classifier. These variables turn out to be quite effective for identifying the bubble wall-layer and the interior zone. On the other hand, the successful classification rate is already high enough for this relatively simple system. We have not observed an obvious change in performance when switching from NN to random forest, or to SVM. However, when the dataset becomes large, the random forest method and SVM take longer computational time compared with the NN classifier. Thus, we choose the artificial neural network as the classification tool.

Figure 5.8 shows the performance, as measured by ROC curve and confusion matrix on the training, testing, validation and overall data set. This re-sampling strategy, by dividing the data into several groups, is the same as the a priori test done in previous chapters. In the confusion matrix, the green part shows if the classifier successfully tells the data within class 1 (data inside wall-layer) from class 2 (data inside interior-region), while the red part means that the NN misclassified the class 1 data as class 2 or vice versa. Take the training dataset as an example (top left frame of figure 5.8 ). There are a total of 3598 (3712+54+12+315) pieces of data,
containing 327 (12+315) pieces of data from the wall-layer and 3766 (3712+54) pieces of data from the channel interior-region. There are 3712 pieces of data from class 1 successfully classified as class 1, consisting 89.4% of the total dataset. However, 54 pieces of data are misclassified as class 2, which consist of 1.5% of the entire dataset. Thus at the end of the first row, the success rate in classifying class 1 is 98.3%. Similarly in the second row, the success rate in classifying class 2 is 96.3%. Adding the success rate along the diagonal line of the matrix results in an overall success rate of 98.2%.

Based on the confusion matrix, the ROC curve is shown in figure 5.9. The ROC curve is generated by plotting the true positive rate (value at the end of the first row in the confusion matrix) against the false positive rate (value at the end of the second row of the confusion matrix) at various threshold settings. The 45 degree line in figure 5.9 means a random guess, and the more the curve is bending toward the left top corner, the better performance the classifier will have. The confusion matrix and the ROC curve show that, the classifier successfully separates the data using only three quantities (features), which indirectly supported the feasibility of separate modeling in the wall-layer and the interior-region.

Similarly, the feature selection and the a priori test are done separately. In the following figure 5.10, the rank of importance of each variables is plotted for the interior-region. The turbulent kinetic energy becomes much more important, in addition to the mean shear rate, which is still the dominant parameter here, together with $Q$. However, the importance of the variables inside the wall-layer, as plotted in figure 5.11, shows that the turbulent quantities, together with the statistical quantities describing the structure of the interface become more critical, which suggests that additional equations for the interface area evolution may be needed for bubbly flows in this parameter range.
Figure 5.8. The Confusion matrix for the training (top left frame), the validation (top right frame), the testing (bottom left frame) and the overall dataset (bottom right frame). Each confusion matrix records the success classification rate and misclassification rate by comparing the output class (learned model results) with the real target class (DNS results).
Figure 5.9. The ROC curves of both class 1 and class 2 based on the training (top left frame), the validation (top right frame), the testing (bottom left frame) and the overall dataset (bottom right frame). Each ROC curve shows how the true positive rate is related with the false positive rate based on the classification results in each dataset.
Figure 5.10. The rank of importance of each variable inside interior-region based on mean decrease gini index.

Figure 5.11. The rank of importance of each variable inside wall-region based on mean decrease gini index.
Figure 5.12 shows the root mean square error (RMSE) versus the number of variables for the wall-layer (left frame) and interior-region (right frame). Based on the data, the number of variables needed to reconstruct the closure terms remains unchanged at six for both the wall-layer and interior-region. Even though the slope of the leaning curve does not decrease as sharply as when the training was done with the whole data.

Figure 5.13 shows the a priori test inside the wall layer (left frame) and the interior-region (right frame). The fitting performance remains reasonably good using the reduced set of variables in both the wall-layer and the interior-region.

5.3 Expanded dataset for turbulent flows with nearly spherical bubbles

For turbulent Couette flow and Poiseuille flows, large shear rate regions are close to the wall and the steady state vertical velocity profile quickly becomes nearly flat in the channel interior-region. Thus, it is difficult to separate the effect of the wall from the velocity gradient, which is the main factor for the nearly spherical bubble’s horizontal lift force. In order to expand the parameter range for varying shear rates
in the channel interior-region, where the effect of the walls are small, we initialize
the liquid turbulent flow using a moving wall boundary condition together with a
parabolic profile due to an imposed driven pressure to create Couette-Poiseuille (C-
P) type flow as the initial velocity field. The detailed setup used to create different
types of C-P flows can be found in [Pirozzoli, 2011]. By changing the wall velocity
with a specific added driving pressure, steady state turbulent velocity profiles with
different slopes can be generated in the interior-region of the channel.

In this subsection, more data are added to the training dataset to model the
closure terms, in order to make the parameter range less sparse. We have gathered
data for channel Reynolds numbers based on half channel width 6000, 8000 and 9000
for steady C-P single phase flows. This is done by gradually changing the wall velocity
to get different shear rate. Then we insert 20 bubbles and 30 bubbles. The driving
pressure is $\beta = 0.0018$, and the wall velocity ranges from 1.5 to 3.5 in intervals of
0.5.
Figure 5.14. Vertical vorticity iso-surface at magnitude 7 (top frame) and velocity magnitude contour in the middle plan in span-wise z-direction (bottom frame), respectively at time 0.25, 5.5, 12, for turbulent C-P flow with 30 bubbles and moving wall velocity at 2.
Figure 5.15. Evolution of the vertical velocity with bubble void fraction for different training data.
To give the reader a better picture of the data, figure 5.14 shows the iso-surface of vertical vorticity magnitude at 7 and -7 (top 3 frames), as well as vertical velocity magnitude (bottom 3 frames) with 30 bubbles in the C-P channel flow at the mid-plane in the z-direction in one of the training cases. The moving wall velocity is 2. In this case, initially the 30 bubbles are placed in the right hand side of the channel and the channel width is 2. The bubble diameter is 0.2, with $Eo = 0.12$ and $Mo = 2.56 \times 10^{-10}$. The bubbles are nearly spherical and the rise velocity is relatively high, with bubble Reynolds number around 100. Initially most of the vorticity is generated in the wall region. As time goes on, the nearly spherical bubbles migrate towards the left hand side of the channel, and more and more bubble induced vorticity becomes visible in the interior-region. Similar unsteady cases with different shear rate and the void fraction, but the same $Eo$ and Morton number are generated to use as training data. Figure 5.15 shows the evolution of the vertical liquid velocity and the void fraction distribution for six training cases at different times. For the cases with 20 bubbles (left frames in figure 5.15), all the bubbles are nearly uniform between 0.5 and 1.5 in the wall-normal direction, and the moving wall velocities are 1.5, 2.0 and 3.0 respectively. For the cases with 30 bubbles (right frames in figure 5.15), we make the distribution of the bubbles a little skewed, and places all of them nearly uniform between 1.0 and 1.5 in wall-normal direction, and the moving wall velocities are also 1.5, 2.0 and 3.0 respectively. A comparison of the liquid velocities at different times in figure 5.15 shows that, the bubbles have not caused obvious changes to the averaged vertical liquid velocity, except for inducing some small fluctuations. This is as expected because the simulation time is too short for each case to reach a steady state.

The current approach is based on a supervised machine learning, which means that no matter which regression method we use to fit the closure terms, the more comprehensive the training data is, the better the predicting performance will be. We
TABLE 5.1

FEATURE SELECTION WITH DIFFERENT DATASET

<table>
<thead>
<tr>
<th>case</th>
<th>1th</th>
<th>2th</th>
<th>3th</th>
<th>4th</th>
<th>5th</th>
<th>6th</th>
</tr>
</thead>
<tbody>
<tr>
<td>30-2</td>
<td>alpha</td>
<td>k</td>
<td>dk/dx</td>
<td>dv/dx</td>
<td>ω_y</td>
<td>da/dx</td>
</tr>
<tr>
<td>20-2</td>
<td>k</td>
<td>dv/dx</td>
<td>ω_y</td>
<td>Ω</td>
<td>dk/dx</td>
<td>α</td>
</tr>
<tr>
<td>30-3</td>
<td>k</td>
<td>dv/dx</td>
<td>α</td>
<td>da/dx</td>
<td>dk/dx</td>
<td>ω_y</td>
</tr>
<tr>
<td>Combined</td>
<td>k</td>
<td>dk/dx</td>
<td>α</td>
<td>dv/dx</td>
<td>ω_y</td>
<td>da/dx</td>
</tr>
</tbody>
</table>

start with the data from only the cases with spherical bubbles in the interior-regions. For this specific situation, we do not need to run the simulations for a long enough time to reach the steady state to gather the information needed.

The ultimate goal is to train a generalized model that can be used to predict new cases. Based on the different training cases, table 5.1 summarizes the top 6 most important variables in each dataset for $< u'v' >$, as well as in a comprehensive training dataset which combines all six dataset together.

For ideal cases, as more and more dataset with a variety of parameters are added to the training pool, the learning performance should become better or at least be a compromise between those of a “good” training dataset and a “bad” dataset. However, this is not always true. One reason is the noises in the simulation data, especially when the magnitudes of average quantities are close to zero, so the fitting is more like a “0-0” fitting. Another reason is that the unknown closure terms must can be well correlated by the known average quantities. Thus, the closure terms need to be selected cautiously during the feature selection process.

In the table 5.1, we show the $< u'v' >$ term, as an example. The number 30-2 means the case with 30 bubbles and a moving wall velocity of 2. We see that the
ranking of the top six important parameters does not changed much between the datasets, and it is clear which variables are the most critical ones for the modeling.

A comparison of learning curves is plotted in figure 5.16, which shows the decrease of the RMSE versus the number of variables for the $< u'v' >$ term (top frame), the $< u'u' >$ term (middle frame) and $dp/dx$ term (bottom frame). For the Reynold stresses $< u'v' >$ and $< u'u' >$, when different training dataset are combined together, the RMSE decreases much faster as the first three to four key variables are gradually included, and finally reaches a small value compared with the results from modeling each training dataset separately. For the pressure gradient term $< dp/dx >$, the learning performance is a compromise between those of the separate training cases.

5.4 Turbulent flows with topology change

Although much of our work on DNS of multiphase flows has focused on bubbly flows, in many cases, particularly if the void fraction is high, the interface topology is much more complex and the interfaces undergo continuous coalescence and breakup.

Modeling such flows is still very primitive and we expect DNS and statistical learning to be able to cast considerable light on the various processes governing such flows.

5.4.1 DNS results of turbulent flows with topology change

We have done several simulations of flows undergoing topology changes. We first work on results for a Poiseuille type flow at a friction Reynolds number of 128. There are 40 bubbles with the same diameter of 0.4 and $Eo = 80$, which makes the total void fraction 13.58%. Evolutions of the bubbles are shown in the figure 5.17. The same average quantities, which are shown in the figure 5.3 for the bubbly flows without topology changes, are plotted below.
Figure 5.16. The model learning curve for the $<u'v'>$ term (top frame), the $<u'u'>$ term (middle frame) and the $dp/dx$ term (bottom frame), based on training on different datasets.
Figure 5.17. The evolution of flow with topology changes. Several bubbles are initially places in a turbulent channel flow. The surface tension is sufficiently low so the bubbles break up, after the initial coalescence.

Figure 5.18. Evolution of averaged quantities. The profiles are shown at time 10, 55, 80 and 100 for bubbly flow with topology changes.
Figure 5.19. Distribution of averaged area concentration (top left frame) and the interface projection area $A_x$ in the stream-wise direction (top right frame), the interface projection area $A_y$ in the wall-normal direction (bottom left frame), and the interface projection area $A_z$ in the span-wise direction (bottom right frame), at time 10, 55, 80 and 100 for bubbly flow with topology changes.

Figure 5.20. Evolution of total averaged area concentration and its three direction projections from time 0 to 100.
In figures 5.18 we show several quantities averaged over planes parallel to the walls versus the horizontal coordinate at four times (10, 55, 80 and 100, all in computational units). It is clear that the average velocity has not changed much presumably, due to the deformable bubble being trapped in the interior-region. As the flow evolves further, deformable bubbles stay in the interior-region and therefore do not increase the shear rate at the wall. The turbulent shear, $\langle u'v' \rangle$, is plotted versus the horizontal coordinate in the 3th row first column of figure 5.18. For both the turbulent kinetic energy and the Reynolds stress terms, there is an initial decrease in magnitude before time 55, followed by an increase as time evolves to 100. This is likely to be caused by the bubble’s breakup after the initial coalescence. In figures 5.19 we plot the statistical information of the interface areas averaged over planes parallel to the walls, which includes the total area concentration ($A$), as well as the evolution of the projection areas respectively on stream-wise ($A_x$), wall-normal ($A_y$) and span-wise ($A_z$) directions, versus the wall-normal coordinate, at four different times.

Figures 5.20 shows the evolution of the total averaged area concentration and its three direction projections from time 0 to 100. The total area concentrations are the integrals over the wall-normal direction of each of the quantities plotted in figure 5.19, at each time. The total interface area keeps increasing up to the time 50 or so, and then decrease a little bit until it reaches a relatively steady state. Area concentrations in all directions at time 55 are obviously large than those at time 10, as is seen both in figure 5.19 and figure 5.20. This can be caused by the bubble’s initial coalescence and stretch under the effect of the liquid shear rate. However at time 80, the magnitude of the total area concentration decreases a little bit compared with time 40, and this can be caused by bubble breakup. For bubbly flow with topology changes, for this parameter range, we believe that the interface information is becoming increasingly critical for the turbulent closure terms modeling, and this will be discussed in details in the next section on feature selection.
5.4.2 Turbulent feature selection

While some questions remain about how the detailed modeling of the coalescence influences the results, we are starting to examine how DNS results can help with the modeling of such flows. Results from a recursive feature selection are shown in the next two figures, for the average lateral gas flux.

Figure 5.21 shows the mean decrease gini index for each variable in the case with topology changes. Notice that the order of the variables is different than for the bubbly flows without topology changes. Among the top 6 most important variables, the area concentrations are more important compared with previous case without topology changes shown in figure 5.6.

Figure 5.22 shows the root-mean square error (RMSE) versus the number of variables included. The error decreases and the correlation coefficient increases rapidly with the number of variables and after about six variables, there are only minor changes. This is similar to what we saw for the bubbly flow without topology change.

Figure 5.21. The mean decrease gini index for the various variables used to describe the horizontal gas flux for flow with topology changes.
In this specific parameter range, not only the rank of importance for each variable has changed, but the slope of the decrease of the RMSE also becomes less steeper as variables are gradually added, as is also seen in figure 5.22.

5.4.3 A priori tests for closure terms

To assess how well the gas fluxes are predicted by the most important variables for the case with topology changes, we have used a neural network to relate the fluxes and the selected variables. Figure 5.23 shows the flux predicted by the model versus the DNS data. In the top two frames we use the training data set but in the bottom two frames we explore how well the first six variables in figure 5.21 describe the flux for the test data set. In this a priori test, the fitting performance still remains relatively high, similar to the results for the case without topology changes.
Figure 5.23. The model prediction versus the DNS data for the full (top) and the reduced (bottom) dataset. The training data is on the left and the test data on the right.
5.5 Conclusion

Here we examine that how DNS results can be used to model turbulent channel bubbly flow continuing the studies of laminar flows in chapter 4. We have done this in the context of a relatively simple setup for both Poiseuille and the Couette-Poiseuille type flow, following the transient evolution of bubbly flow in a vertical channel, with and without topology changes.

There are several topics covered in this chapter. Those include the turbulent feature selection for the closure terms, a priori test with the DNS data for the closure terms’ fitting, identification of bubbly wall layer and interior-region, and methods to make a more comprehensive training dataset. The preliminary results are promising and robust. Once we determine the evolution equations for the turbulent bubbly system based on the current study, the proposed work is to validate the predictive performance of the turbulent modeling, as those done in previous chapters.
CHAPTER 6

CONCLUSIONS

Direct Numerical Simulations (DNS) of multiphase flows have seen rapid progress over the last decade, and high-fidelity simulations have generated a tremendous amount of data. However, attempts to use DNS results to help modeling of multiphase flows are still rare. Meanwhile, for most industrial and natural systems, DNS requires too fine grid resolution to be practical. Since the small scale behavior often exhibits significant universality, it is likely that the small scales can usually be modeled, rather than fully resolved. For many purposes a low order description of the system, such as the average motion, is all that is needed. In this thesis, we have run simulations of bubbly flows in vertical channels, for both laminar and turbulent cases. These DNS results are used to help develop, validate and verify a reduced order model for the average, or the large-scale, bubbly flow.

As a first step, we have examined the use of neural networks to fit DNS data to develop closure relations for the average two-fluid equations in a very simple, fully periodic bubble system. Overall, the average equations with the neural network closure almost perfectly reproduce the main aspects of the DNS results, including the generally rapid change initially as well as the level of unsteadiness remaining after the initial adjustment. While it can be argued that the present problem is sufficiently simple so that success is likely, we feel that the small size of the training data and the relatively high level of fluctuations observed in the DNS results resulted in better agreement than we expected.
The approach taken here allows us to continue exploring the uncertainty of the model and how it depends on the sampling of the training data. The model is then trained repeatedly with random sampling and the prediction performances are used for uncertainty quantification. The prediction results show some fluctuations, but the mean value closely following the DNS prediction, and using the trained closures to predict bubbly flows of new situations shows similar results. This shows that the model averaging neural networks, compared with the traditional neural networks, could be a promising method to reduce the uncertainty caused by the training data.

This success of this first step has provided a general work-flow for the later works, although most multiphase flows are considerably more complex than the system considered here, we believe that there is nothing that intrinsically limits using data mining for the closure terms to these systems.

Next, we extend the studies from the full periodic bubbly flow to a wall-bounded case, and examine how DNS results can be used to provide closure relations for the bubbly flow modeling in vertical channels. A transient evolution of bubbly flow in a vertical channel is simulated. We use a model averaging neural network that is trained on one DNS data set and then applied to other situations where the initial velocity, void fraction and boundary conditions are different in the channel, but for which we also have DNS results to compare with. Overall, the average equations with the neural network closure reproduce the main aspects of the DNS results reasonably well, even though not that perfectly, as which does in the fully periodic cases.

We have also found that the closure terms by postulating a relationship with unknown coefficients that are found using linear regression. Both approaches give comparable results, but given the slightly better accuracy and their generality, we believe that the neural networks are the preferred approach for more complex flows.

Finally, we examined how DNS results can be used to model turbulent channel bubbly flow continuing the studies of laminar flows. We have done this in the
context of a relatively simple setup for both Poiseuille and Couette-Poiseuille type flow, following the transient evolution of bubbly flow in a vertical channel, with and without topology changes. Based on these DNS data, we have made a best practice for the turbulent feature selection for the closure terms. Using this feature selection method, combined with the NN's fitting, high correlation rate with fewer input variables can be achieved during the a priori test with the DNS data.

Some additional topics are also covered, including the identification of bubbly wall-layer and interior-region, and methods to generate a more comprehensive training dataset. The preliminary results are promising and robust. Once we determine the evolution equations for the turbulent bubbly system based on the current study, the proposed work is to validate the predictive performance of the turbulent modeling, as those done in the previous chapters.
APPENDIX A

PLANAR AVERAGE OF THE VERTICAL CONSERVATION OF VOLUME EQUATION

We start with
\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \]  (A.1)

Multiply by \( H \) and integrate

\[ \frac{1}{L} \int H \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dy = \frac{1}{L} \int \left( \frac{\partial H u}{\partial x} + \frac{\partial v H}{\partial y} - u \frac{\partial H}{\partial x} - v \frac{\partial H}{\partial y} \right) dy = \frac{\partial}{\partial x} \left( \frac{1}{L} \int H u dy \right) + 0 + \frac{1}{L} \int \mathbf{u} \cdot \nabla H dy = \frac{\partial}{\partial x} \alpha < u > + \frac{\partial \alpha}{\partial t} \]  (A.2)

since \( \mathbf{u} \cdot \nabla H = -\partial H/\partial t \) and we have used the definition of \( \alpha_l \). Thus, the void fraction evolves according to

\[ \frac{\partial \alpha_l}{\partial t} + \frac{\partial}{\partial x} F_l = 0, \]  (A.3)

where

\[ F_l = \frac{1}{L} \int H u dy = \alpha_l < u >. \]  (A.4)

Note also that \( \alpha_b + \alpha_l = 1 \) and \( \alpha_b < u_b > + \alpha_l < u_l > = 0 \), so that \( F_b = -F_l \).
APPENDIX B

PLANAR AVERAGE OF THE VERTICAL MOMENTUM EQUATIONS

We outline the derivation of equation (2.7), which is a simplified version of the general multi fluid momentum equation. To keep the derivation as simple as possible we assume two-dimensional flow in the $x-y$ plane, where the averaging is over the $y$-direction. Averaging the full equations over the $y-z$ plane produces the same results. The $y$-momentum equation, written for the whole flow field.

\[
\frac{\partial \rho v}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial \rho v^2}{\partial y} = -\frac{d\rho_0}{dy} - \frac{\partial p'}{\partial y} - \rho g_y + \frac{\partial}{\partial x}\mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} 2\mu \frac{\partial v}{\partial y}, \quad (B.1)
\]

where we have written the pressure gradient as a sum of the imposed gradient and a periodic perturbation pressure. The density and viscosity of the gas can be taken as zero, so that we can write $\rho = \rho_l H$ and $\mu = \mu_l H$, where

\[
H = \begin{cases} 
1 & \text{in liquid;} \\
0 & \text{in gas.} 
\end{cases} \quad (B.2)
\]

The planar phasic average of the liquid velocity and volume fraction are defined as: $<v>_l = \frac{1}{\alpha_l L} \int Hvdy$, $\alpha_l = \frac{1}{L} \int Hdy$, where $L$ is the period in the $y$ direction.
The average of the left hand side is

\[ \frac{1}{L} \int \left( \frac{\partial \rho \mu H}{\partial t} + \frac{\partial \rho \mu H \nu}{\partial x} + \frac{\partial \rho \mu H \nu^2}{\partial y} \right) dy \]

\[ = \rho \frac{\partial}{\partial t} \frac{1}{L} \int H \nu dy + \rho \frac{\partial}{\partial x} \frac{1}{L} \int H \nu dy + \rho \frac{\partial}{\partial y} \frac{1}{L} \int H \nu^2 dy \]

\[ = \rho \frac{\partial}{\partial t} \alpha_l < v >_t + \rho \frac{\partial}{\partial x} \alpha_l < \nu >_t + 0. \]  

(B.3)

The pressure and the gravity terms are

\[ \frac{1}{L} \int \left( \frac{d \rho_o}{dy} + \frac{\partial \rho'}{\partial y} + \rho_i H g_y \right) dy = \frac{d \rho_o}{dy} + 0 + \rho_i g_y \alpha_l. \]  

(B.4)

The average of the viscous term is:

\[ \frac{1}{L} \int \left( \frac{\partial}{\partial x} \mu_i H \left( \frac{\partial \nu}{\partial x} + \frac{\partial \nu}{\partial y} \right) + \frac{\partial}{\partial y} \left( 2 \mu_i H \frac{\partial \nu^2}{\partial y} \right) \right) dy \]

\[ = \frac{\partial}{\partial x} \left( \frac{\mu_i}{L} \int H \left( \frac{\partial \nu}{\partial x} + \frac{\partial \nu}{\partial y} \right) dy \right) + \frac{1}{L} \left[ 2 \mu_i H \frac{\partial \nu^2}{\partial y} \right]_0 = \left( \frac{\partial}{\partial x} \left( \frac{\mu_i}{\mu_l} \left( \frac{\partial \nu}{\partial x} + \frac{\partial \nu}{\partial y} \right) \right) \right)_t \]

\[ = \frac{\partial}{\partial x} \left( \mu_l \frac{\partial^2}{\partial x^2} \left( \alpha_l < v >_t \right) \right) + 0 - \frac{\partial}{\partial x} \left( \mu_i \int \left( \frac{\partial H}{\partial x} + \frac{\partial H}{\partial y} \right) dy \right) \]  

(B.5)

If we decompose the velocity field into a mean and fluctuation part, \( u_l = < u >_t + u'_l \), and \( v_l = < v >_t + v'_l \), and use that

\[ \frac{\partial \alpha}{\partial x} = \frac{1}{L} \int \frac{\partial H}{\partial x} dy, \]  

(B.6)
the viscous term is:

$$\mu \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) - \frac{\partial}{\partial x} \left( \mu \int (\langle v >_l + u'_l) \frac{\partial H}{\partial x} + (\langle u >_l + u'_l) \frac{\partial H}{\partial y} \right) dy $$

$$= \mu \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) - \frac{\mu}{L} \frac{\partial}{\partial x} \left( < v >_l \int \frac{\partial H}{\partial x} dy + < u >_l \int \frac{\partial H}{\partial y} dy \right) $$

$$+ \int \left( v'_l \frac{\partial H}{\partial x} + u'_l \frac{\partial H}{\partial y} \right) dy $$

$$= \mu \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) - \mu \frac{\partial}{\partial x} \left( < v >_l \frac{\partial \alpha}{\partial x} + \frac{1}{L} \int (v'_l n_x + u'_l n_y) \delta dy \right) $$

$$= \mu \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) + \mu \frac{\partial}{\partial x} \left( < v >_l \frac{\partial \alpha}{\partial x} \right) -$$

$$\mu \frac{\partial}{\partial x} \left( < v >_l \frac{\partial \alpha}{\partial x} + \frac{1}{L} \int (v'_l n_x + u'_l n_y) \delta dy \right) $$

$$= \mu \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) - \frac{\mu}{L} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y). \quad (B.7)$$

Here we use that $\frac{\partial H}{\partial x} = \delta n_x$, and $\frac{\partial H}{\partial y} = \delta n_y$, where $\delta$ is a delta function and $n_x, n_y$ are the normal components of the normal vector. The summation in the last line of equation (16) is over the interfaces (bubble surfaces that cross the $x = constant$ plane), using the equation above, the averaged equation for the vertical momentum is:

$$\rho_l \frac{\partial}{\partial t} \alpha_l < v >_l + \rho_l \frac{\partial}{\partial x} \alpha_l < u v >_l$$

$$= -\frac{dp_o}{dy} - \rho_l g_y \alpha_l + \frac{\mu}{L} \frac{\partial}{\partial x} \alpha_l \frac{\partial < v >_l}{\partial x} - \frac{\mu}{L} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y). \quad (B.8)$$
Dividing by the liquid density, and introducing the kinematic viscosity \( \nu_l = \mu_l/\rho_l \),
gives:

\[
\frac{\partial}{\partial t} \alpha_l < v >_l + \frac{\partial}{\partial x} \alpha_l < uu >_l \bigg|_{y} = -\frac{1}{\rho_l} \frac{dp_o}{dy} - g_y \alpha_l + \nu_l \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) - \frac{\nu_l}{L} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y). \tag{B.9}
\]

If we write \(< uu >_l = < uu >_l < v >_l + < u'u' >_l \) and ignore the fluctuating interface viscous terms, we have

\[
\frac{\partial}{\partial t} \alpha_l < v >_l + \frac{\partial}{\partial x} \alpha_l < uu >_l \bigg|_{y} = -\frac{1}{\rho_l} \frac{dp_o}{dy} - g_y \alpha_l + \nu_l \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) - \frac{\partial}{\partial x} \alpha_l < uu' >_l. \tag{B.10}
\]

Here, we have ignored

\[
\frac{\nu_l}{L} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y). \tag{B.11}
\]

In the fully periodic case, we have left out the surface tension term in the derivation above. For spherical bubbles it is easily shown that the average of this term zero. The average of the \(y\)-component is

\[
\frac{1}{L} \int \sigma_k n_y \delta dy = \frac{1}{L} \sigma_k \sum_{int} n_y = \frac{1}{L} \sigma_k \sum_{bub} (n_{y}^{top} + n_{y}^{bot}). \tag{B.12}
\]

which is zero, since for a spherical bubble \( n_{y}^{top} = -n_{y}^{bot} \). However, due to the deformation of the spherical bubbles approaching the walls, surface tension term is no more trivial, and we treat it as one of the unknown closures as well.
APPENDIX C

PLANAR AVERAGE OF THE HORIZONTAL MOMENTUM EQUATIONS

We start by the $x$-momentum equation, written for the whole flow field

$$
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial y} = -\frac{\partial p'}{\partial x} + \frac{\partial}{\partial x} \left( 2\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right),
$$

and assume again that the density and viscosity of the gas can be taken as zero, so that we can write $\rho = \rho_t H$ and $\mu = \mu_t H$. The average of the left hand side is

$$
\frac{1}{L} \int \left( \frac{\partial \rho_t H u}{\partial t} + \frac{\partial \rho_t H u^2}{\partial x} + \frac{\partial \rho_t H uv}{\partial y} \right) dy
$$

$$
= \rho_t \frac{\partial}{\partial t} \frac{1}{L} \int Hudy + \rho_t \frac{\partial}{\partial x} \frac{1}{L} \int Hu^2 dy + \rho_t \frac{\partial}{\partial y} \frac{1}{L} \int Hu dy
$$

$$
= \rho_t \frac{\partial}{\partial t} \alpha < u >_t + \rho_t \frac{\partial}{\partial x} \alpha < uu >_t + 0.
$$

To average the pressure gradient, notice that it is zero in the bubbles if $\rho = \mu = 0$ there. Thus, we can write

$$
\frac{1}{L} \int \frac{\partial p}{\partial x} dy = \frac{1}{L} \int H \frac{\partial p}{\partial x} dy = \alpha_t \left< \frac{\partial p}{\partial x} \right>_t
$$

We may want to check that the first and second averages indeed are the same.
The average of the viscous term, using that \( \mu = \mu_i H \), is:

\[
\frac{1}{L} \int \left( \frac{\partial}{\partial x} 2\mu_H \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} \mu_H \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right) dy \\
= \frac{\partial}{\partial x} \left( \frac{2\mu_i}{L} \int H \frac{\partial u}{\partial x} dy \right) + \frac{\mu_i}{L} \left[ H \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right]_0^L = \frac{2\mu_i}{L} \frac{\partial}{\partial x} \left( \int H \frac{\partial u}{\partial x} dy \right) \\
= \frac{2\mu_i}{L} \frac{\partial}{\partial x} \left( \int \left( \frac{\partial u H}{\partial x} - \frac{u}{\partial x} \frac{\partial H}{\partial x} \right) dy \right) = 2\mu_i \frac{\partial^2}{\partial x^2} \alpha_l < u > - \frac{2\mu_i}{L} \frac{\partial}{\partial x} \left( \int \left( \frac{\partial u}{\partial x} \frac{\partial H}{\partial x} \right) dy \right) \\
= 2\mu_i \frac{\partial}{\partial x} \left( \alpha_l < u > \frac{\partial}{\partial x} \right) - \frac{2\mu_i}{L} \frac{\partial}{\partial x} \left( \int u \frac{\partial H}{\partial x} dy \right) \\
+ 2\mu_i \frac{\partial}{\partial x} \left( < u > \frac{\partial \alpha_l}{\partial x} \right) - \frac{2\mu_i}{L} \frac{\partial}{\partial x} \left( \int \frac{\partial H}{\partial x} dy \right) \\
= 2\mu_i \frac{\partial}{\partial x} \alpha_l \frac{\partial < u >}{\partial x} - \frac{2\mu_i}{L} \frac{\partial}{\partial x} \sum u' n_y \quad \text{(C.4)}
\]

Gathering the terms, we have

\[
\rho_l \frac{\partial}{\partial t} \alpha_l < u > + \rho_l \frac{\partial}{\partial x} \alpha_l < uu > \\
- \alpha_l \left( \frac{\partial p}{\partial x} \right)_l + 2\mu_i \frac{\partial}{\partial x} \alpha_l \frac{\partial < u >}{\partial x} - 2\mu_i \frac{\partial}{\partial x} \sum u' n_y + (f_x)_x \quad \text{(C.5)}
\]

Writing \( u = < u > + u' \), the advection term is

\[
\alpha_l < uu > = \alpha_l < ( < u > + u')^2 > = \\
\alpha_l < u >^2 + \alpha_l < u'u' > = < u > F_l + \alpha_l < u'u' > \quad \text{(C.6)}
\]

\[
\frac{\partial F_l}{\partial t} + \frac{\partial}{\partial x} < u > F_l = \\
- \alpha_l \left( \frac{\partial p}{\partial x} \right)_l + 2\mu_i \frac{\partial}{\partial x} \alpha_l \frac{\partial < u >}{\partial x} - \frac{2\mu_i}{L} \frac{\partial}{\partial x} \sum u' n_y + \frac{1}{\rho_l} (f_x)_x - \frac{\partial}{\partial x} \alpha_l < uu > \quad \text{(C.7)}
\]

The main unknown in this equation is the pressure force, which can be interpreted as the lift force.
APPENDIX D

PLANAR AVERAGE OF THE VERTICAL MOMENTUM EQUATIONS WITH 3D VERSION

To keep the derivation as simple as possible we assume two-dimensional flow in the $x-y$ plane, where the averaging is over the $y$-direction. Averaging the full equations over the $y-z$ plane produces the same results. The $y$-momentum equation, written for the whole flow field,

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial \rho v^2}{\partial y} + \frac{\partial \rho vw}{\partial z} = -\frac{d\rho_0}{dy} - \frac{\partial \rho'}{\partial y} - \rho g_y +$$

$$\frac{\partial}{\partial x} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial y} + \frac{\partial}{\partial z} \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right)$$

where we have written the pressure gradient as a sum of the imposed gradient, $\frac{d \rho_0}{dy}$, and a periodic perturbation pressure, $\frac{\partial \rho'}{\partial y}$. The density and viscosity of the gas can be taken as zero, so that we can write $\rho = \rho_l H$ and $\mu = \mu_l H$, where

$$H = \begin{cases} 
1 & \text{in liquid;} \\
0 & \text{in gas.}
\end{cases} \quad (D.1)$$

The planar phasic average of the liquid velocity and volume fraction are defined as:

$$<v>_l = \frac{1}{\alpha_l A} \iiint H v d\gamma d\zeta, \quad \alpha_l = \frac{1}{A} \iiint H d\gamma d\zeta,$$

where $A$ is the area of $y-z$ plane. The
average of the left hand side is

\[
\frac{1}{A} \int \int \left( \frac{\partial \rho_l H v}{\partial t} + \frac{\partial \rho_l H uv}{\partial x} + \frac{\partial \rho_l H v^2}{\partial y} + \frac{\partial \rho_l H vw}{\partial z} \right) dydz
\]

\[
= \rho_l \frac{\partial}{\partial t} \frac{1}{A} \int \int H v dydz + \rho_l \frac{\partial}{\partial x} \frac{1}{A} \int \int H uv dydz
\]

\[
+ \rho_l \frac{\partial}{\partial y} \frac{1}{A} \int \int H v^2 dydz + \rho_l \frac{\partial}{\partial z} \frac{1}{A} \int \int H vw dydz
\]

\[
= \rho_l \frac{\partial}{\partial t} \alpha_l < v >_l + \rho_l \frac{\partial}{\partial x} \alpha_l < uv >_l + 0 + 0.
\] (D.2)

The pressure and the gravity terms are

\[
\frac{1}{A} \int \int \left( \frac{dp_0}{dy} + \frac{\partial p'}{\partial y} + \rho_l H g_y \right) dydz = \frac{dp_0}{dy} + 0 + \rho_l g_y \alpha_l.
\] (D.3)

The average of the viscous term is:

\[
\frac{1}{A} \int \int \left( \frac{\partial \mu_l H (\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}) + \frac{\partial}{\partial y} 2\mu_l H \frac{\partial v}{\partial y} + \frac{\partial}{\partial z} \mu_l H (\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y})} dydz
\]

\[
= \frac{\partial}{\partial x} \left( \frac{\mu_l}{A} \int \int H (\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}) dydz \right) + \frac{1}{A} \int \int \left[ 2\mu_l H \frac{\partial v}{\partial y} \right]_0^L dz
\]

\[
+ \frac{\partial}{\partial z} \left( \frac{\mu_l}{A} \int \int H (\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}) dydz \right)
\]

\[
= \frac{\partial}{\partial x} \left( \frac{\mu_l}{A} \int \int (\frac{\partial H v}{\partial x} + \frac{\partial H u}{\partial y} - v \frac{\partial H}{\partial x} - u \frac{\partial H}{\partial y}) dydz + 0
\]

\[
+ \frac{\partial}{\partial z} \left( \frac{\mu_l}{A} \int \int (\frac{\partial H w}{\partial z} + \frac{\partial H v}{\partial y} - v \frac{\partial H}{\partial z} - w \frac{\partial H}{\partial y}) dydz
\]

\[
= \mu_l \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) + 0 - \frac{\partial}{\partial x} \left( \frac{\mu_l}{A} \int \int (v \frac{\partial H}{\partial x} + u \frac{\partial H}{\partial y}) dydz \right)
\]

\[
+ 0 - \frac{\partial}{\partial z} \left( \frac{\mu_l}{A} \int \int (v \frac{\partial H}{\partial z} + w \frac{\partial H}{\partial y}) dydz \right).
\]

If we decompose the velocity field into a mean and fluctuation part, \( u_l = < u >_l + u'_l \), \( v_l = < v >_l + v'_l \) and \( w_l = < w >_l + w'_l \), and use that

\[
\frac{\partial \alpha}{\partial x} = \frac{1}{A} \int \int \frac{\partial H}{\partial x} dydz,
\] (D.4)
the viscous term is:

\[
\mu_i \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) - \frac{\partial}{\partial x} \left( \frac{\mu_i}{A} \int \int (\langle v >_l + v'_l) \frac{\partial H}{\partial x} + \langle u >_l + u'_l) \frac{\partial H}{\partial y} \right) dydz
\]

\[- \frac{\partial}{\partial z} \left( \frac{\mu_i}{A} \int \int (\langle v >_l + v'_l) \frac{\partial H}{\partial z} + (\langle w >_l + w'_l) \frac{\partial H}{\partial z} \right) dydz \]

\[= \mu_i \frac{\partial^2}{\partial x^2} (\alpha_l < v >) - \mu_i \frac{\partial}{\partial x} \left( \langle v >_l \frac{\partial H}{\partial x} \right) \int \int dydz + \int \int (\langle v >_l \frac{\partial H}{\partial x} + \langle u >_l \frac{\partial H}{\partial y} \right) dydz \]

\[= \mu_i \frac{\partial^2}{\partial x^2} (\alpha_l < v >_l) - \mu_i \frac{\partial}{\partial x} \left( \langle v >_l \frac{\partial H}{\partial x} \right) + \frac{1}{A} \int \int (v'_l n_x + u'_l n_y) \delta dydz \]

\[\mu_i \frac{\partial}{\partial z} \left( \frac{1}{A} \int \int (v'_l n_x + w'_l n_y) \delta dydz \right) \]

\[= \mu_i \frac{\partial}{\partial z} \left( \alpha_l \frac{\partial}{\partial x} \right) + \mu_i \frac{\partial}{\partial x} \left( \langle v >_l \frac{\partial H}{\partial x} \right) \]

\[- \mu_i \frac{\partial}{\partial x} \left( \langle v >_l \frac{\partial H}{\partial x} + \frac{1}{A} \int \int (v'_l n_x + u'_l n_y) \delta dydz \right) \]

\[- \mu_i \frac{\partial}{\partial z} \left( \frac{1}{A} \int \int (v'_l n_x + w'_l n_y) \delta dydz \right) \]

\[= \mu_i \frac{\partial}{\partial x} (\alpha_l \frac{\partial}{\partial x}) - \mu_i \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y) - \mu_i \frac{\partial}{\partial z} \sum_{int} (v'_l n_z + w'_l n_y). \quad (D.5) \]

Here we use that \( \frac{\partial H}{\partial x} = \delta n_x, \frac{\partial H}{\partial y} = \delta n_y \) and \( \frac{\partial H}{\partial z} = \delta n_z \), where \( \delta \) is a delta function and \( n_x, n_y \) and \( n_z \) are the normal components of the normal vector. The summation in the last line of equation (D.6) is over the interfaces (bubble surfaces that cross the \( x = constant \) plane), using the equation (D.2), (D.3), (D.6), the averaged equation
for the vertical momentum is:

\[
\rho_l \frac{\partial}{\partial t} \alpha_l < v >_l + \rho_l \frac{\partial}{\partial x} \alpha_l < uv >_l = -\frac{dp_0}{dy} - \rho_l g_y \alpha_l + \mu_l \frac{\partial}{\partial x} \alpha_l \frac{\partial < v >_l}{\partial x} - \\
\frac{\mu_l}{A} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y) - \frac{\mu_l}{A} \frac{\partial}{\partial z} \sum_{int} (v'_l n_z + w'_l n_y).
\]  

(D.6)

Dividing by the liquid density, and introducing the kinematic viscosity \( \nu_l = \mu_l / \rho_l \),
gives:

\[
\frac{\partial}{\partial t} \alpha_l < v >_l + \frac{\partial}{\partial x} \alpha_l < uv >_l = -\frac{1}{\rho_l} \frac{dp_0}{dy} - g_y \alpha_l + \nu_l \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) - \\
\frac{\nu_l}{A} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y) - \frac{\nu_l}{A} \frac{\partial}{\partial z} \sum_{int} (v'_l n_z + w'_l n_y).
\]  

(D.7)

If we write \( < uv >_l = < u >_l < v >_l + < u'v' >_l \) and ignore the fluctuating interface viscous terms, we have

\[
\frac{\partial}{\partial t} \alpha_l < v >_l + \frac{\partial}{\partial x} \alpha_l < u >_l < v >_l = -\frac{1}{\rho_l} \frac{dp_0}{dy} - g_y \alpha_l + \nu_l \frac{\partial}{\partial x} \left( \alpha_l \frac{\partial < v >_l}{\partial x} \right) - \frac{\partial}{\partial x} \alpha_l < u'v' >_l.
\]  

(D.8)

Here, we have ignored

\[
\frac{\nu_l}{A} \frac{\partial}{\partial x} \sum_{int} (v'_l n_x + u'_l n_y) + \frac{\nu_l}{A} \frac{\partial}{\partial z} \sum_{int} (v'_l n_z + w'_l n_y),
\]  

(D.9)

as done in Appendix B.
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