LA-UR-17-29883
Approved for public release; distribution is unlimited.

Title: Uncertainty Quantification of Multi-Phase Closures

Author(s): Nadiga, Balasubramanya T.
Baglietto, Emilio

Intended for: Report

Issued: 2017-10-27

Uncertainty Quantification of Multi-Phase Closures (L3 Milestone THM.CLS.P15.09)

B.T. Nadiga
Computational Physics Group (CCS-2)
Los Alamos National Laboratory
Los Alamos, NM 87544

E. Baglietto
Nuclear Sicence & Engineering
MIT, Cambridge, MA 02139

1 Executive Summary

In the ensemble-averaged dispersed phase formulation used for CFD of multiphase flows in nuclear reactor thermohydraulics, closures of interphase transfer of mass, momentum, and energy constitute, by far, the biggest source of error and uncertainty. Reliable estimators of this source of error and uncertainty are currently non-existent. Here, we report on how modern Validation and Uncertainty Quantification (VUQ) techniques can be leveraged to not only quantify such errors and uncertainties, but also to uncover (unintended) interactions between closures of different phenomena. As such this approach serves as a valuable aide in the research and development of multiphase closures.

The joint modeling of lift, drag, wall lubrication, and turbulent dispersion—forces that lead to tranfer of momentum between the liquid and gas phases—is examined in the framework of validation of the adiabatic but turbulent experiments of Liu and Bankoff, 1993. An extensive calibration study is undertaken with a popular combination of closure relations and the popular $k-\epsilon$ turbulence model in a Bayesian framework. When a wide range of superficial liquid and gas velocities and void fractions is considered, it is found that this set of closures can be validated against the experimental data only by allowing large variations in the coefficients associated with the closures. We argue that such an extent of variation is a measure of uncertainty induced by the chosen set of closures. We also find that while mean fluid velocity and void fraction profiles are properly fit, fluctuating fluid velocity may or may not be properly fit. This aspect needs to be investigated further.

The popular set of closures considered contains ad-hoc components and are undesirable from a predictive modeling point of view. Consequently, we next consider improvements that are being developed by the MIT group under CASL and which remove the ad-hoc elements. We use non-intrusive methodologies for sensitivity analysis and calibration (using Dakota) to study sensitivities of the CFD representation (STARCCM+) of fluid velocity profiles and void fraction profiles in the context of Shaver and Podowski, 2015 correction to lift, and the Lubchenko et al., 2017 formulation of wall lubrication.

2 Introduction

The method of choice for modeling dispersed Eulerian multiphase flow as occurs in nuclear reactors is to ensemble average the mass, momentum, and energy conservation equations for each of the individual phases and then solve the resultant ensemble-averaged equations (e.g., see Drew and Passman, 2006) for each of the phases after using closure relations to represent transfer of mass, momentum, and energy between the different phases. For further details on the formulation and the setup, the reader is referred to Nadiga et al. (2016). Unless otherwise mentioned, STARCCM+'s (see User-Guide, 2016) Eulerian dispersed-multiphase CFD solver is used for this purpose.

The Dakota software toolkit (Adams et al., 2016,) provides a range of capabilities for exploration and design of computational simulations—in this case multiphase simulations using STARCCM+. It contains algorithms for optimization, uncertainty quantification, sensitivity analysis, and model calibration. It further provides a flexible and extensible interface to these methods, enabling them to be applied in an iterative, black box fashion to arbitrary simulation codes—here STARCCM+. CASL report includes demonstrative examples of using Dakota as a harness to conduct UQ, SA, and calibration studies of multiphase flow simulations in STARCCM+.

3 Flow dependency of closure coefficients as a measure of closure error

As mentioned in the summary section, in the ensemble-averaged dispersed phase formulation used for CFD of multiphase flows in nuclear reactor thermohydraulics, closures of interphase transfer of mass, momentum, and energy constitute, by far, the biggest source of error and uncertainty. Nevertheless, reliable estimators of this source of error and uncertainty are currently non-existent. In this section, we show how modern Validation and Uncertainty Quantification (VUQ) techniques can be leveraged to quantify such errors and uncertainties.

We consider a popular set of multiphase closures and then undertake Bayesian calibration of the closure for a series of experiments considered by Liu and Bankoff, 1993 in which the fluid and gas superficial velocities are varied. For each of these cases, Bayesian calibration produces a multi-dimensional posterior distribution of closure coefficients that fits the experimental measurements in a probablistic fashion. When these posterior distributions themselves are combined to form a hyper distribution, the spread in the hyper distribution with flow conditions (here the superficial liquid and gas velocities) can be viewed as a measure of error in the closures. Indeed the spread of this hyper-distribution will be larger than the spread in each of the individual cases and when this extended parameteric uncertainty is propagated through the model at the different flow conditions, the deviation of the mean of the quantities of interest from the corresponding experimental measurements and the increased spread of these responses further serve to characterize the error of the closures.

In this study, we consider the lift force to be parameterized as

$$F_l = C_l \alpha \rho \left[\mathbf{u}_r \times (\boldsymbol{\nabla} \times \mathbf{u}_f) \right], \tag{3.1}$$

following (Auton et al., 1988), the drag force to be parameterized as

$$\begin{aligned} F_d &= \frac{C_d}{2} \rho |\mathbf{u}_r| \mathbf{u}_r \frac{iad}{4} \\ iad &= \frac{6\alpha}{d_b} \\ C_d = f_d C_{d\infty} &= \frac{4}{3} \frac{\Delta\rho}{\rho} \frac{g d_b (1-\alpha)}{u_t^2} \end{aligned} \tag{3.2}$$

and 'a' wall lubrication force to be parameterized as

$$F_{wl} = max \left[0, C_{wl1} + C_{wl2} \frac{r_b}{y_w} \right] \alpha \rho \frac{u_r^2}{d_b} \mathbf{n} \tag{3.3}$$

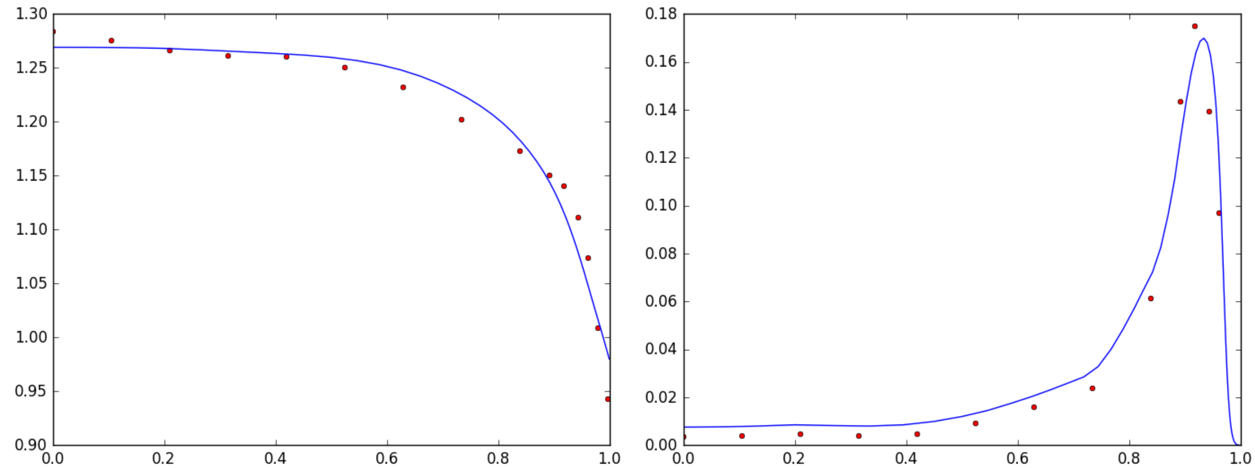

Figure 1: An example model solution using the two-fluid model with lift, drag, and wall lubrication parameterizations of inter-phase momentum transfer. In red are shown measurements of Liu and Bankoff, 1993 for their test case 30 that corresponds to a fluid superficial velocity (J_f) of 1.087 m/s, a gas superficial velocity (J_g) of 0.067 m/s, and a void fraction of 4.073%.. Reasonable comparison of the model solution with measurements verifies the use of the two-fluid model and parameterizations used and leads us to consider further calibration of the model.

following (Antal et al., 1991) We further assume $C = 1/4$ following (Stuhmiller, 1977).

The parameters in the problem then include the axial pressure gradient in the fluid phase $\frac{\partial p}{\partial z}$, and the lift, drag, and wall lubrication coefficients, C_l, C_d, C_{wl1}, and C_{wl2}, besides fluid-phase properties density ρ, and dynamic viscosity μ, the bubble diameter d_b. and the pipe radius r_{max}. The problem specification is completed with a specification of boundary conditions corresponding to symmetry at the axis ($r = 0$), no slip at the wall for the fluid phase, and the channel-average void fraction.

3.1 Liu Bankoff Case 30: J_f=1.087 m/s; J_g=0.067 m/s

Although our main multiphase fluid solver is STARCCM+, and we have carried out numerous UQ studies in STARCCM+ with the help of Dakota, in order to demonstrate the utility of comprehensive Bayesian analysis of multiphase closures as an aide in research and development of such closures, and as discussed in Nadiga et al. (2016), a standalone solver was deemed necessary and initiated in FY16. We have not augumented this solver with the $k - \epsilon$ turbulence model. Figure 1 shows a comparison of the radial profiles of fluid velocity (left) and void-fraction (right) with the experimental measurements of Liu and Bankoff, 1993 for their test case 30 that corresponds to a fluid superficial velocity (J_f) of 1.087 m/s and a gas superficial velocity (J_g) of 0.067 m/s. Figure 2 shows other quantities of interest for this case: the turbulent kinetic energy (TKE), the dissipation rate, the turbulent viscosity, and the ratio of production to dissipation of TKE.

3.2 Spread of closure coefficients

As mentioned previously, a measure of uncertainty of the closure can be quantified by estimating the extent of variation in the closure coefficient for the different flow conditions when this variation is viewd in a hierarchical fashion. Figure 3 shows the ranges of variations

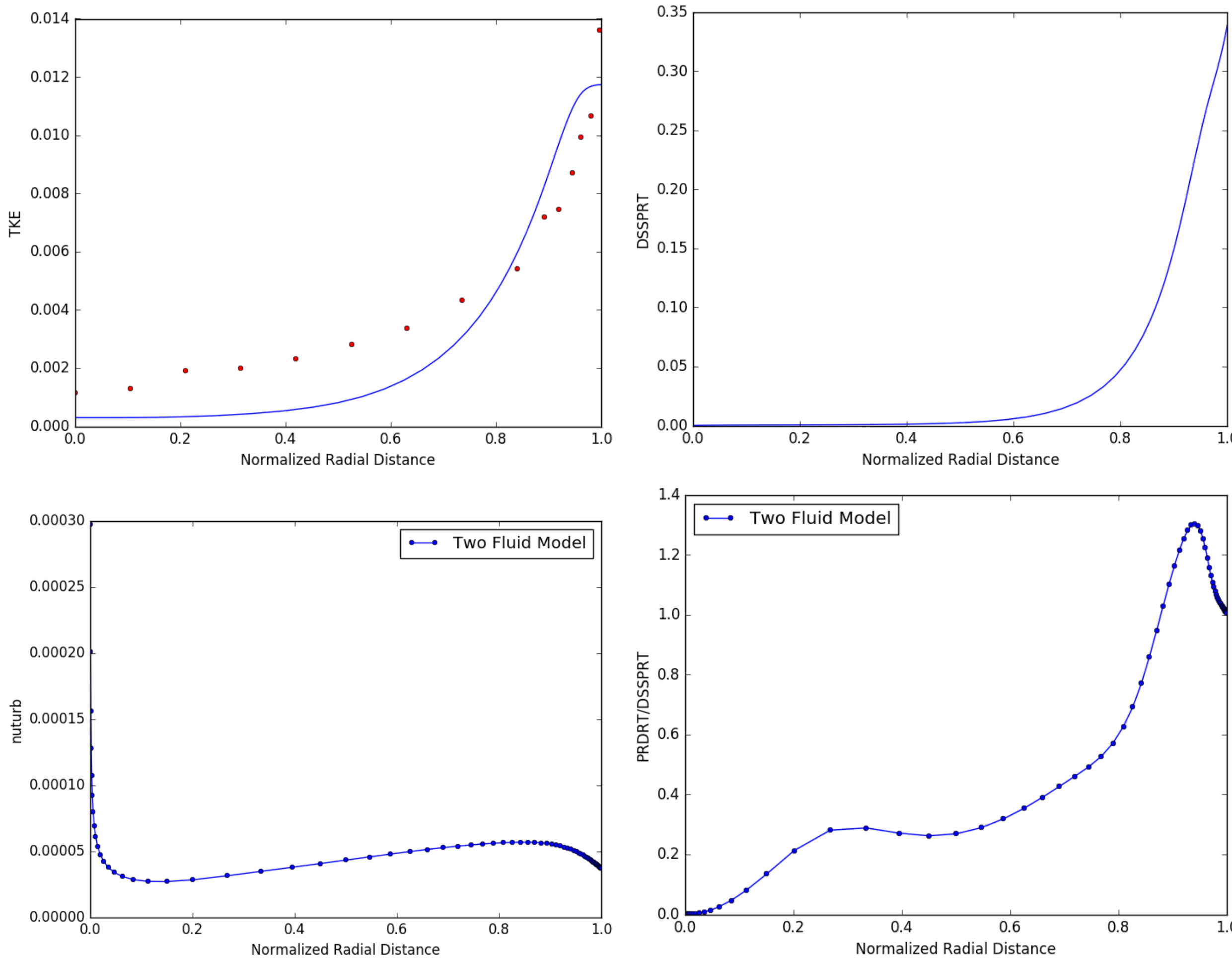

Figure 2: Turbulent kinetic energy, dissipation rate, turbulent viscosity and the ration of production to dissipation of turbulent kinetic energy are shown for the same case as in Fig. 1. (Case 30 of Liu and Bankoff, 1993 with a fluid superficial velocity (J_f) of 1.087 m/s, a gas superficial velocity (J_g) of 0.067 m/s, and a void fraction of 4.073%.). The reasonable correspondance of the turbulent kinetic energy verifies the use of the standard $k-\epsilon$ turbulence model.

in the value of the coefficient of lift needed to fit the individual flow conditions which here consisted of varitions in the superficial gas and liquid velocities. The variations in the quantities of interest that are obtained when such uncertainty in the coefficient of lift and other parameters are propagated through the model are shown in figures 3-5. Further hierarchical analysis of the variation in the values of the closure coefficient lead to an estimate of the uncertainty associated with the closure relations.

4 Analysis of Improved Closures

The popular set of closures considered in the above study contains ad-hoc components and are undesirable from a predictive modeling point of view. Consequently, we next consider improvements that are being developed by the MIT group under CASL and which remove the ad-hoc elements: Baglietto et al., 2013 find that a constant lift coefficient of 0.025 in the context of small spherical bubbles works reasonably. For this reason, we consider a constant lift coefficient that is then damped to zero in the near-wall region using the Shaver and Podowski, 2015 correction (e.g. see Marfaing et al. (2017)):

$$C_L = \begin{cases} 0, & \frac{y}{D_B} < \frac{1}{2} \\ C_{L0}\left(3\left(\frac{2y}{D_B} - 1\right)^2 - 2\left(\frac{2y}{D_B} - 1\right)^3\right), & \frac{1}{2} \leq \frac{y}{D_B} \leq 1 \\ C_{L0}, & \frac{y}{D_B} > 1 \end{cases} \tag{4.4}$$

Next, a more physical development of turbulent dispersion can be found in Burns, 2004, and we adopt that. Finally, a more physics-based formulation of wall-lubrication has been developed in Lubchenko et al., 2017 . In this formulation, wall lubrication force is modeled using an expression derived through an analytical regularization of turbulent dispersion in the near-wall region to account for the decreasing cross-sectional area of the bubbles:

$$F_{wl} = \frac{3}{4} C_D \left(1 + \frac{\alpha}{1-\alpha}\right) \frac{\mu_t U_r}{\sigma_{TD} D_B} \frac{\alpha}{y} \frac{0.5 D_B - y}{D_B - y} \tag{4.5}$$

As pointed out in Marfaing et al. (2017), in contrast to previous methods which interpreted the lubrication force as a physical force pushing bubbles away from the wall, this formulation simply accounts for the geometrical constraint that leads to a reduction of the gas volume fraction away from $y = D_B/2$ towards the wall (assuming spherical bubbles); that is, spherical bubbles touching the wall would naturally lead to the void fraction decreasing monotonically from a radius of the bubble away from the wall towards the wall. As such, this formulation does not introduce tunable coefficients related to wall lubrication. This improved set of closures were implemented in STARCCM+.

As mentioned previously, a measure of uncertainty of the closure can be quantified by estimating the extent of variation in the closure coefficient for the different flow conditions when this variation is viewd in a hierarchical fashion.

To illustrate this approach in a simple setting, we set out to characterize the dependence of this set of closures on the lift coefficient alone. We set this study up as a calibration exercise in which the STARCCM+ rendition of the radial profiles of each of void fraction, fluid velocity, and gas velocity are calibrated simultaneously against the experimental measurements of Liu and Bankoff, 1993. Here the sum-of-squares (L_2) norm was used and the calibration exercise suggests a value of 0.077 for the lift coefficient with a confidence interval of (0.050, 0.102).

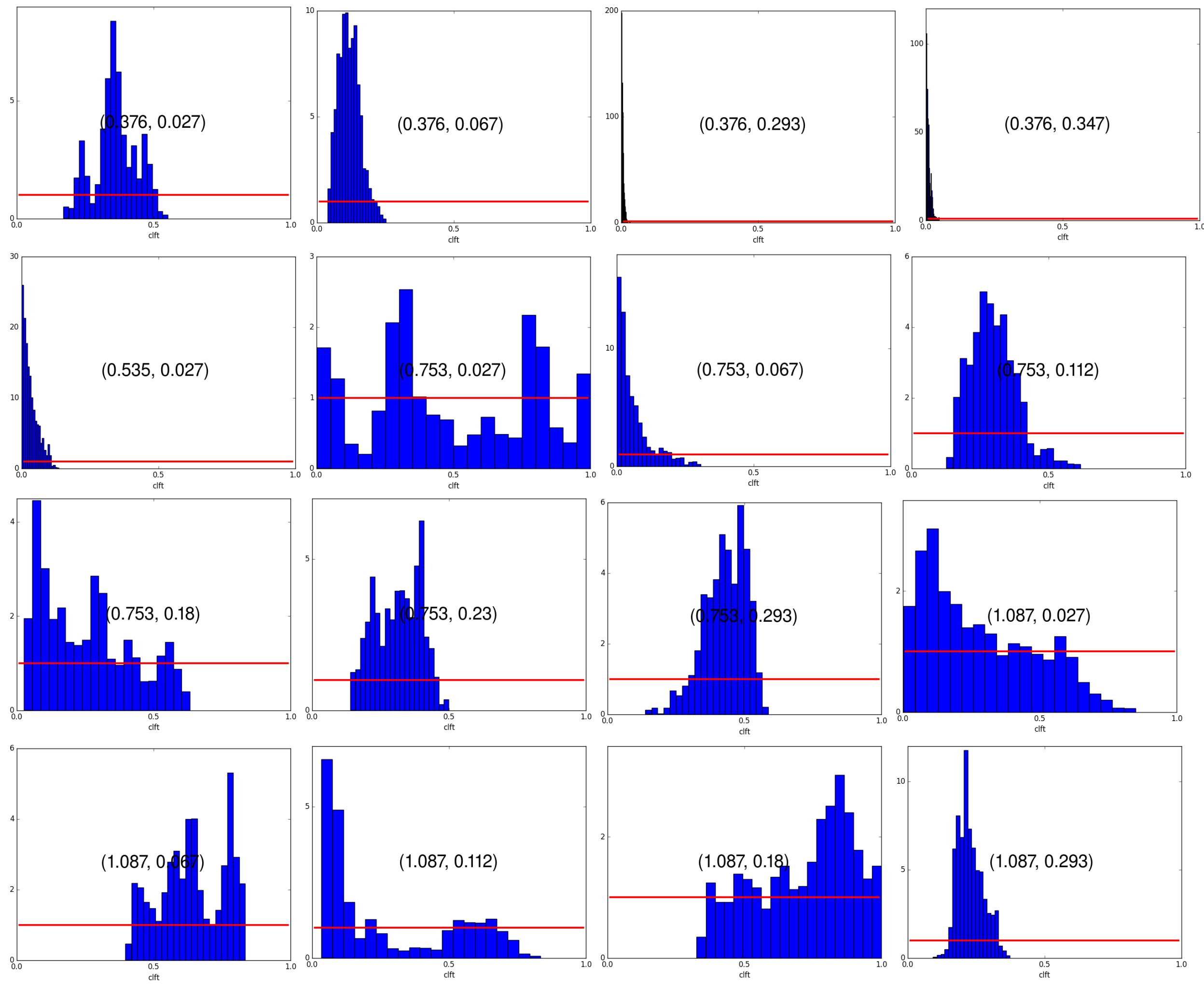

Figure 3: A large fraction of the 42 flow conditions considered in Liu, 1989 is subjected to individual Bayesian calibration. Here the posterior distribution of the lift coefficient for 16 of the cases is shown. The highly nonlinear nature of the equations leads to non-Gaussian distributions of the lift coefficient while noting that considering much longer MCMC chains will likely lead to smoother posteriors. The main observation is that the coefficients of the closure terms vary over wide ranges of values in order to fit the full range of flow conditions. Using kernel density estimates and further hierarchical analysis, the quantification of this spread of closure coefficients is a measure of error/uncertainty in the closure.

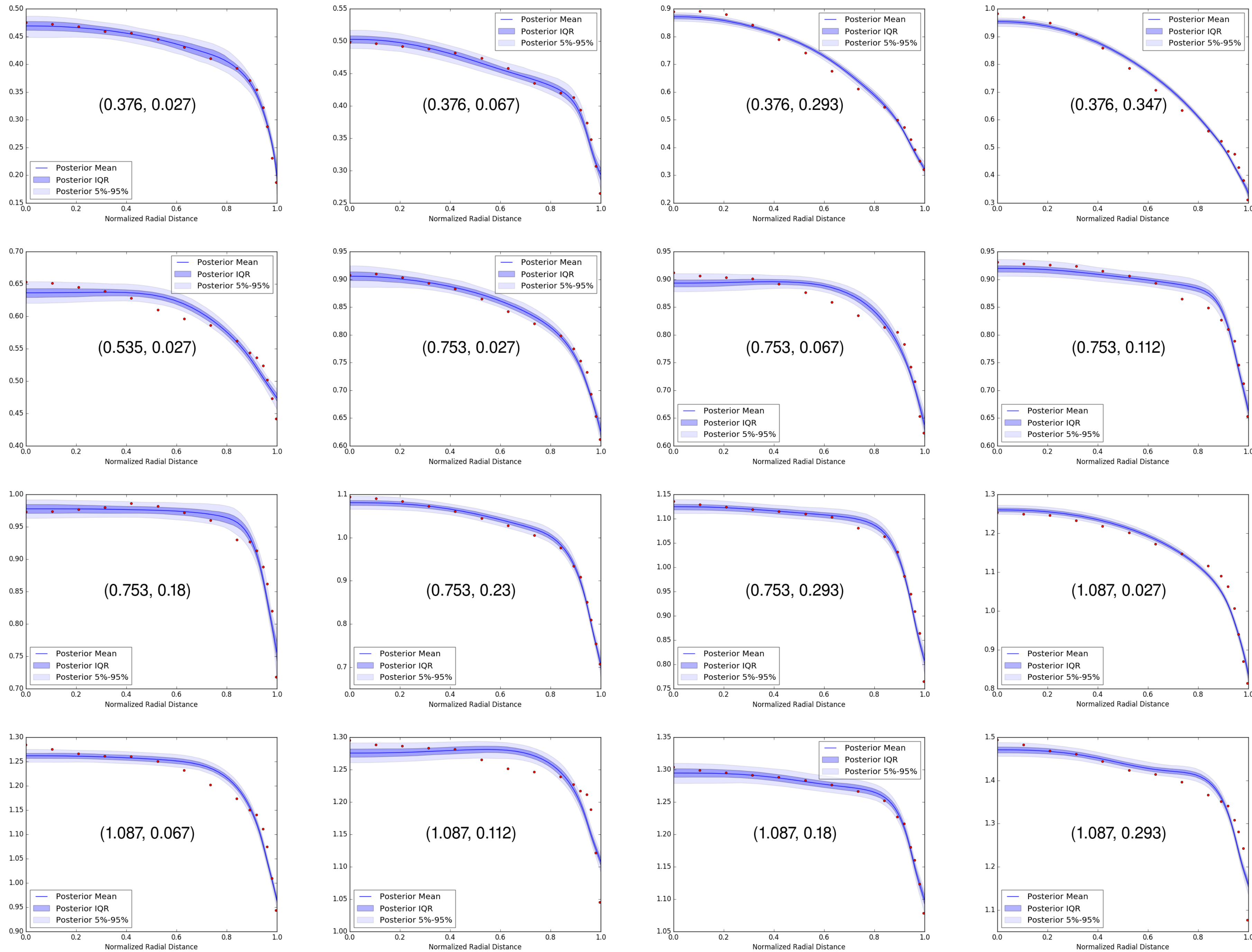

Figure 4: The posterior distributions of closure coefficients are propagated through the two fluid model to obtain uncertainty in the quantities of interest. Here the radial profiles of fluid velocity along with the interquartile range and 90% confidence intervals are shown in blue for the same 16 cases. Experimental data are indicated in red.

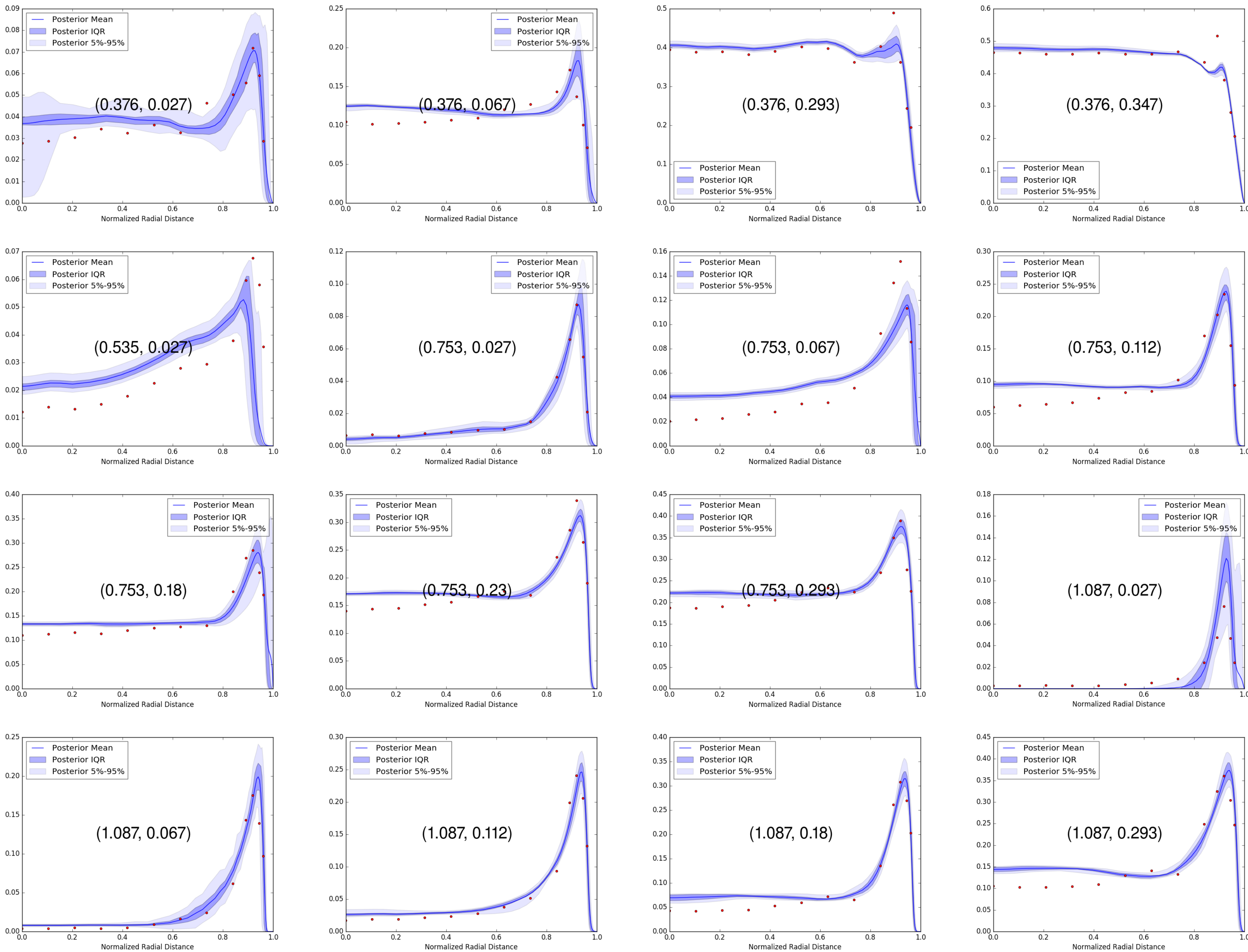

Figure 5: Same as in Fig. ??. Here the radial profiles of void fraction are shown.

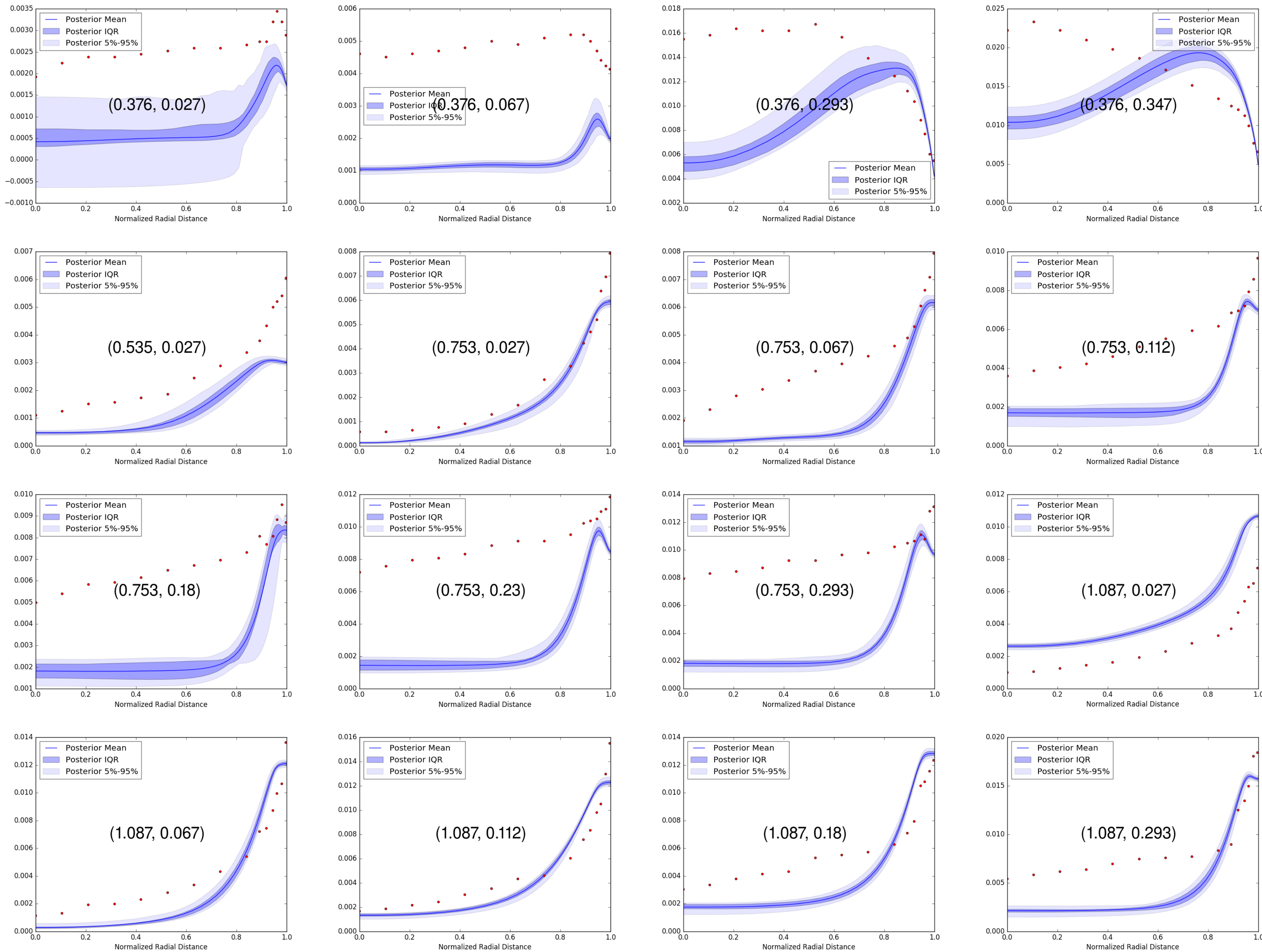

Figure 6: Same as in Fig. ??. Here the radial profiles of gas velocity are shown.

What we mean by a hierarchical analysis here is as follows: We considered 12 of the 42 flow conditions considered in the experiments of Liu, 1989. For this, we chose the smallest and the largest fluid superficial velocities and the full range of gas superficial velocities for these two sets. In the first set of calibrations each of the 12 flow conditions were individually calibrated to obtain a set of 12 values (and ranges) for the lift coefficient. In the second calibration study, all 12 flow conditions were pooled and calibrated to obtain one lift coefficient with a range for the confidence interval. Next, the dispersion of the 12 individual ranges about the single pooled estimate gives us a measure of uncertainty in the closure relations considered.

However, after repeated experimentation with Dakota, it was found that the calibration study did not move the value of the coefficient of lift significantly beyond the inital value of 0.025. We note here that the likely explanation for this behavior is that the local nl2sol method that was used led to an over-emphasis of or essentially getting stuck in a local minimum close to the initial value of the coefficient. For this reason, the results of these experiments are not shown here. However, these results highlight the insufficiency of local methods and implicate the necessity of global and sampling methods to quantify uncertainty in closures.

Given this situation, we conduct a study of the dependence of the flow profiles on the value of the coefficient of lift. While various measures of such sensitivity can be studied like in the previous milestone report, here we think it best to directly show the dependence of the quantities of interest on the value of the coefficient of lift.

For brevity, we show only the void fraction and fluid velocity profiles as obtained in STARCCM+ at a range of lift coefficients for just a few cases in figures 8 through 12. These results suggest that a value of coefficient of lift higher than 0.025 provides a better fit of the experimental measurements for a majority of the cases and that at the higher values of the coefficient of lift, the sensitivity to the coefficient of lift is small. Nevertheless, it remains, e.g., as seen in Fig. 13, that when liquid superficial velocities are low and that of gas is high, i.e, void fraction is high, such higher values of the coefficient of lift lead to a failure of convergence suggesting that a low value for the lift coefficient may be a reasonable compromise.

5 Summary

Uncertainty introduced by closure models in ensemble-averaged Eulerian multiphase approaches have not received much attention. Such uncertainty includes both parameteric uncertainty and model form uncertainty. In this work, we have highlighted how modern Validation and Uncertainty Quantification techniques can be leveraged to quantify such uncertainties in one new fashion. Nevertheless, there are other approaches that need to be developed so as to characterize simulation results with respect to model form uncertainty. We expect to further develop such methods in future work to bring to bear such methods as an aide in further developement of multiphase closures.

References

Adams, B. M., Ebeida, M. S., Eldred, M., Jakeman, J., Maupin, K., JA, M., Swiler, L., Stephens, J., Vigil, D., TM, W., Bohnhoff, W., Dalbey, K., Eddy, J., Hooper, R., Hu, K., Hough, P. D., and EM, R. (2016). Dakota, a multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity

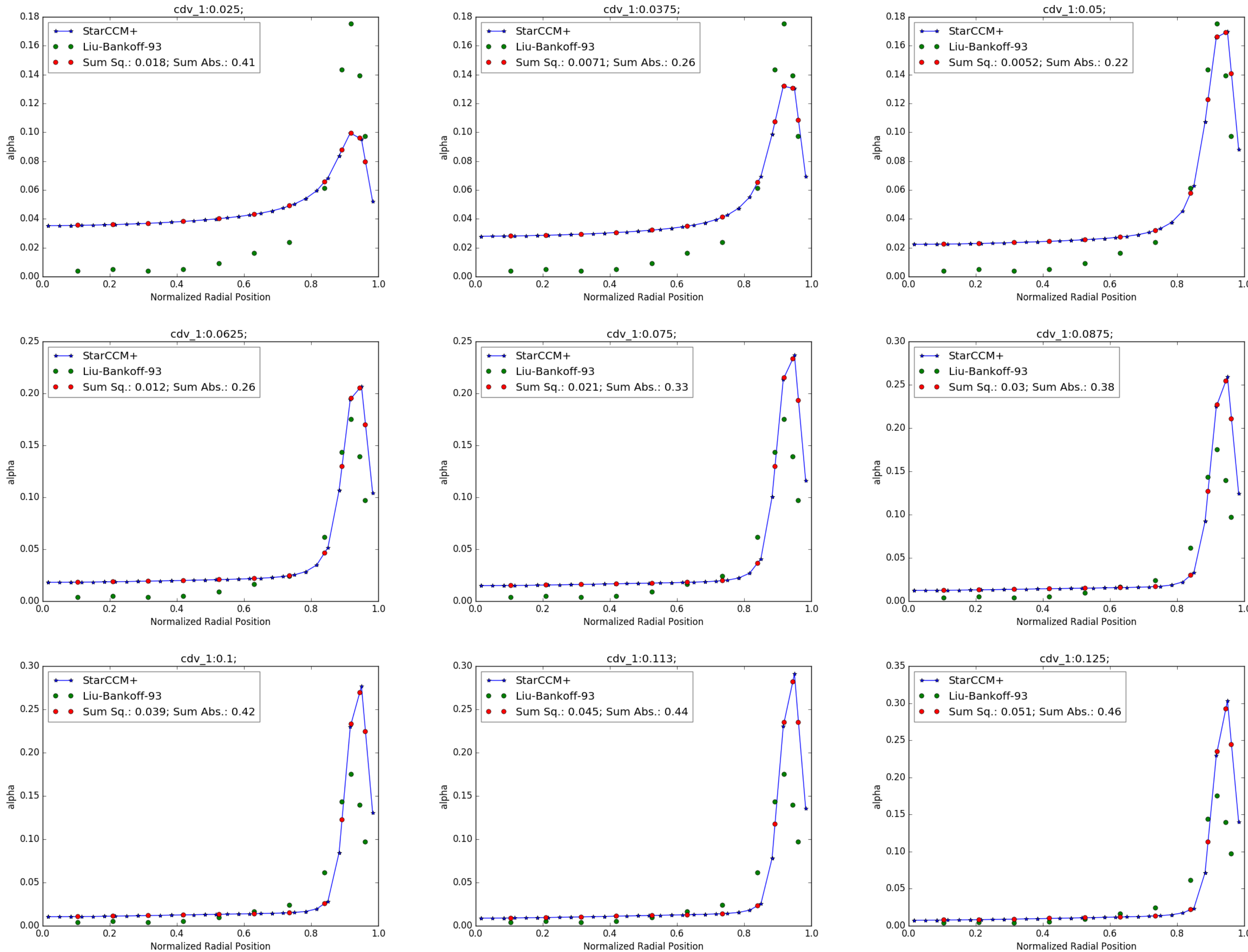

Figure 7: Dependence of void fraction profile on lift coefficient. J_f=1.087 m/s; J_g=0.067 m/s; average void fraction of 4.073%

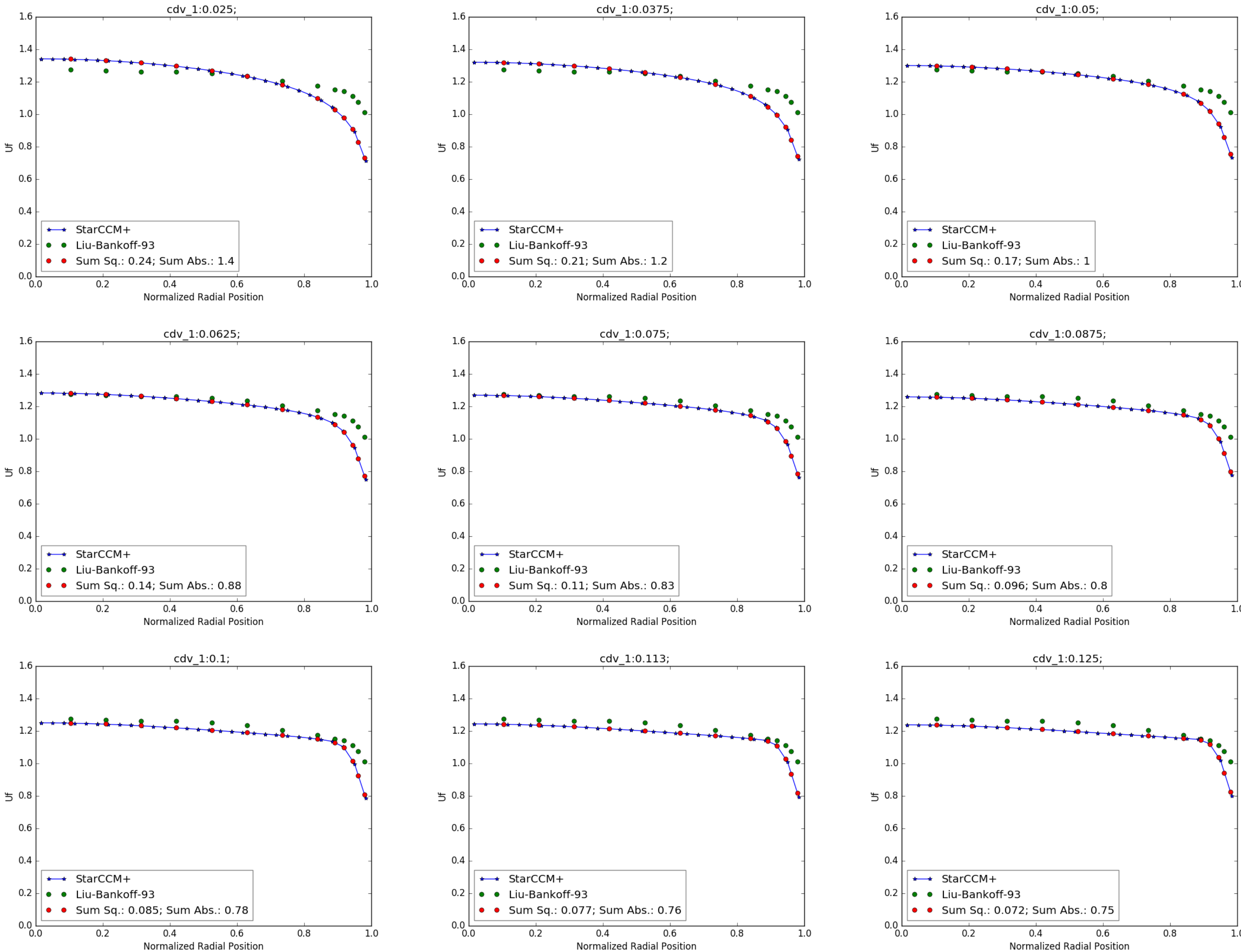

Figure 8: Dependence of fluid velocity profile on lift coefficient. J_f=1.087 m/s; J_g=0.067 m/s; average void fraction of 4.073%

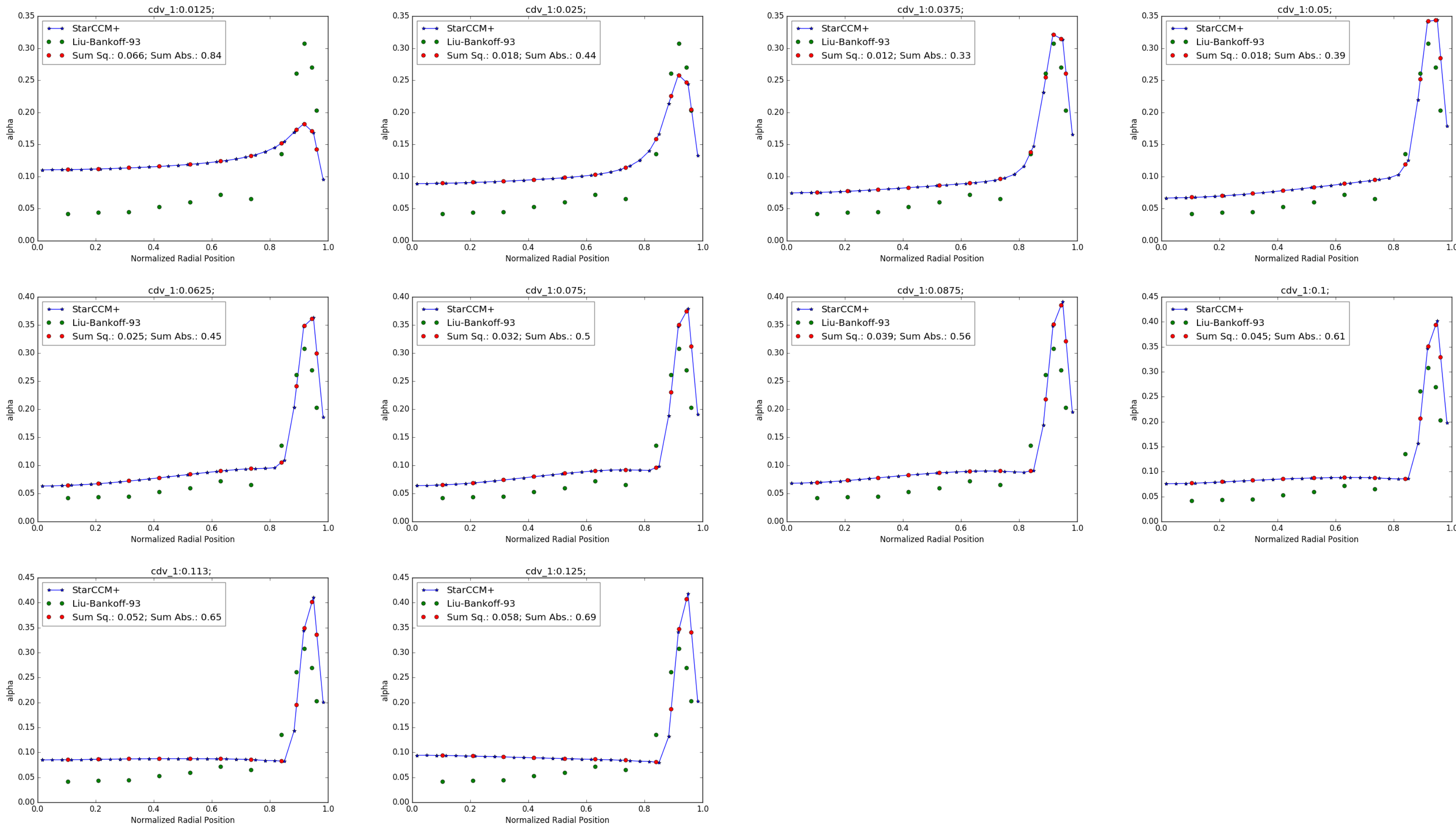

Figure 9: J_f=1.087 m/s; J_g=0.180 m/s; average void fraction of 10.96%

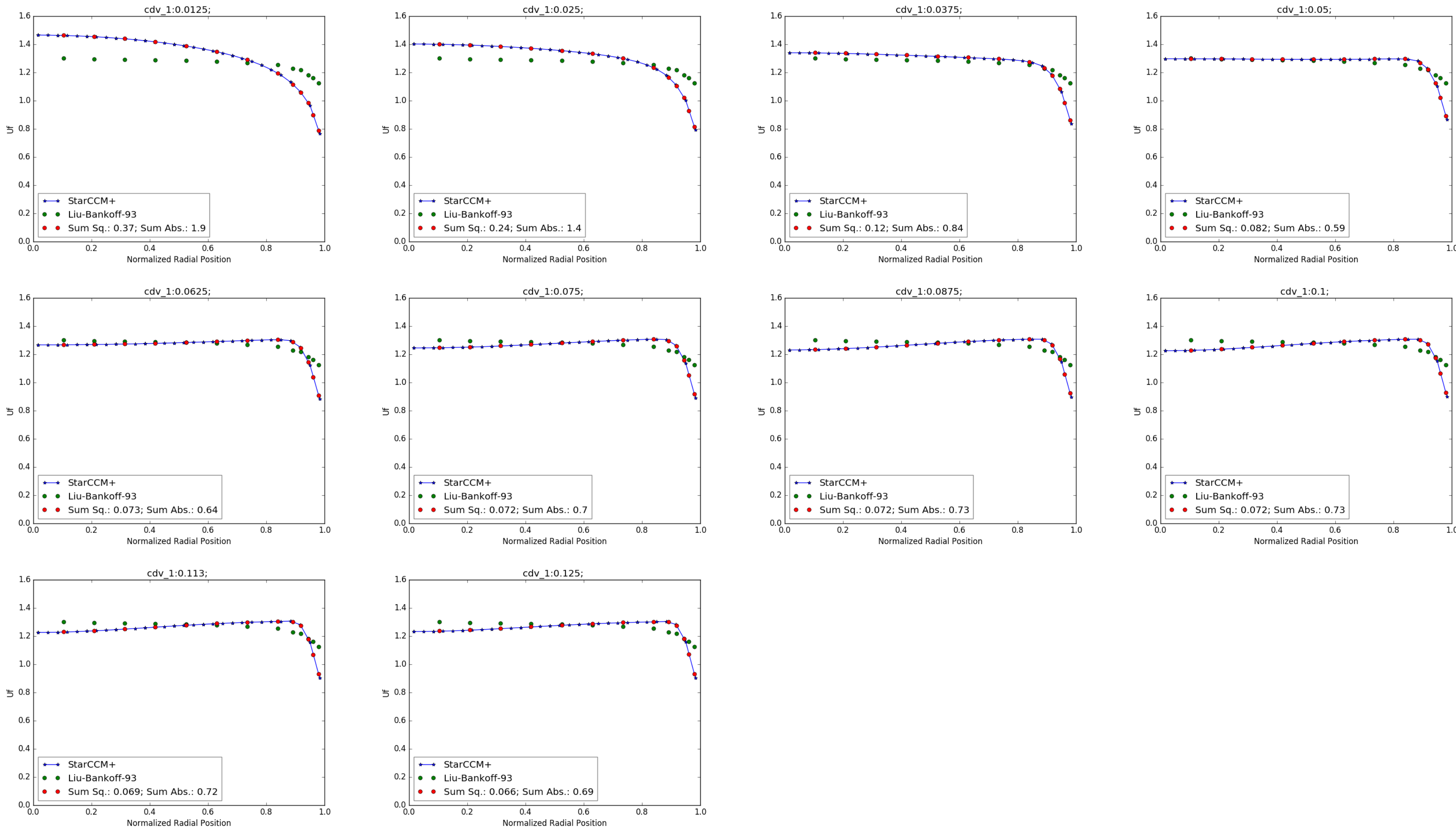

Figure 10: J_f=1.087 m/s; J_g=0.180 m/s; average void fraction of 10.96%

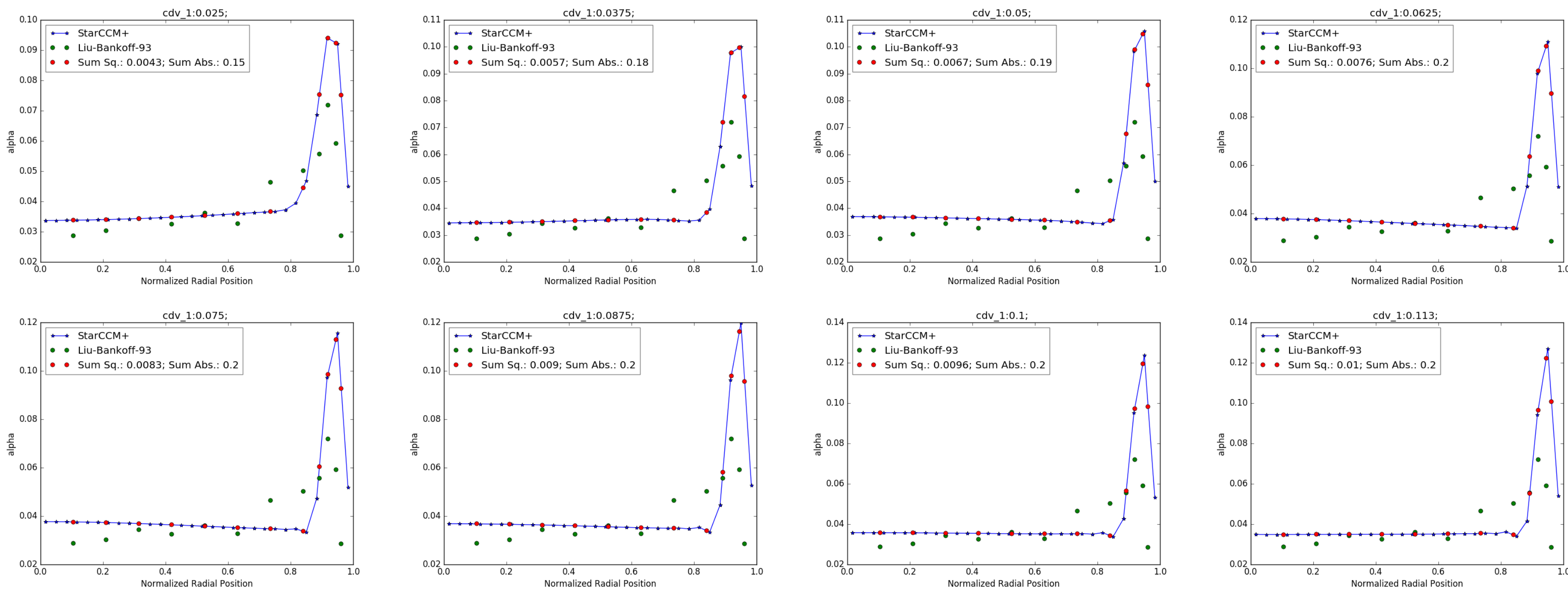

Figure 11: J_f=0.376 m/s; J_g=0.027 m/s; average void fraction of 4.07%

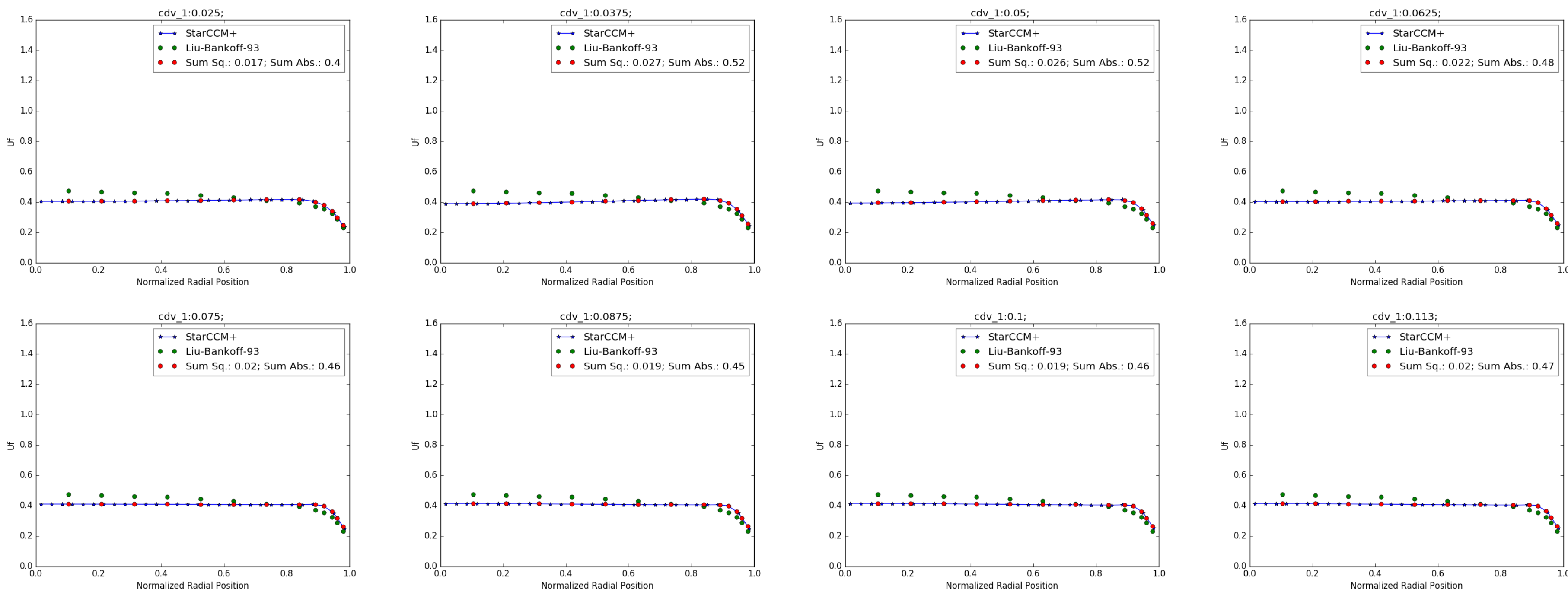

Figure 12: J_f=0.376 m/s; J_g=0.027 m/s; average void fraction of 4.07%

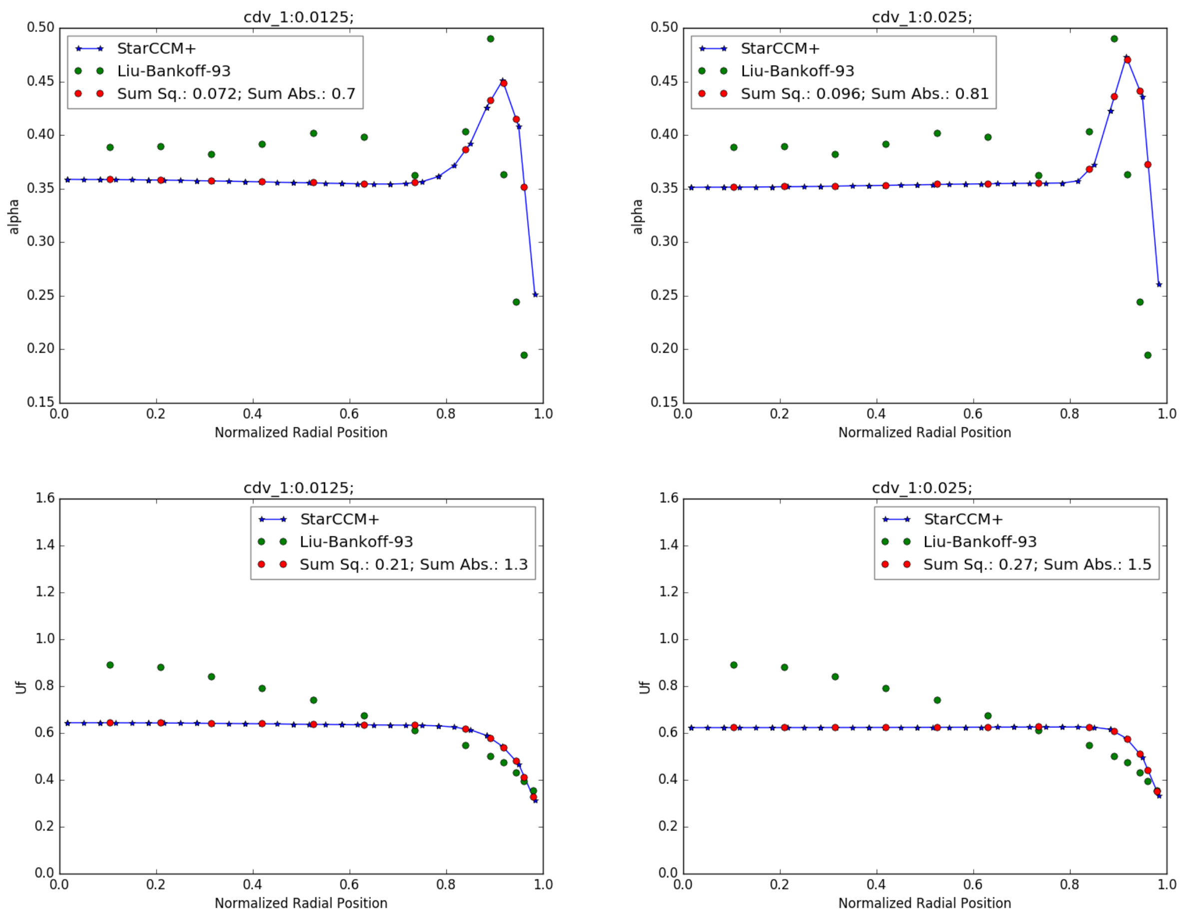

Figure 13: J_f=0.376 m/s; J_g=0.293 m/s; average void fraction of 36.57%

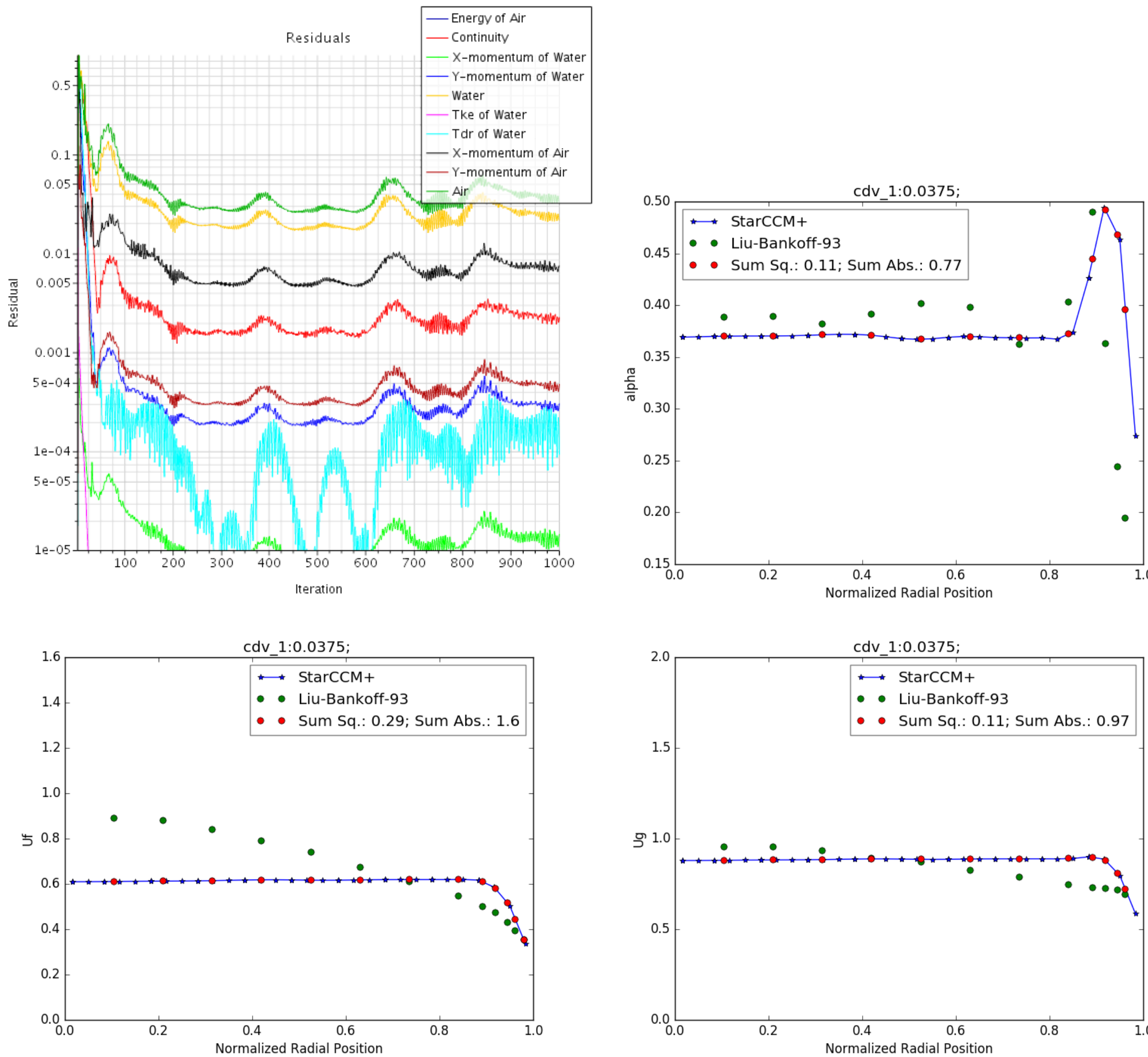

Figure 14: At larger lift coefficients, when the void fraction is high, there were issues of convergence with STARCCM+ as in this example (J_f=0.376 m/s; J_g=0.293 m/s; average void fraction of 36.57%). Note, however, that the fit to experimental data was no worse than in cases that did not have issues with lack of convergence, e.g., as in fig. **??**.

analysis: Version 6.4 user's manual. *Sandia National Laboratories, Tech. Rep. SAND2014-4633*.

Antal, S., Lahey, R., and Flaherty, J. (1991). Analysis of phase distribution in fully developed laminar bubbly two-phase flow. *International Journal of Multiphase Flow*, 17(5):635–652.

Auton, T., Hunt, J., and Prud'Homme, M. (1988). The force exerted on a body in inviscid unsteady non-uniform rotational flow. *Journal of Fluid Mechanics*, 197:241–257.

Drew, D. A. and Passman, S. L. (2006). *Theory of multicomponent fluids*, volume 135. Springer Science & Business Media.

Liu, T. and Bankoff, S. (1993). Structure of air-water bubbly flow in a vertical pipei. liquid mean velocity and turbulence measurements. *International Journal of Heat and Mass Transfer*, 36(4):1049–1060.

Lubchenko, N., Magolan, B., Sugrue, R., and Baglietto, E. (2017). A more fundamental wall lubrication force from turbulent dispersion regularization for multiphase cfd applications. submitted to the international journal of multiphase flow. *preprint*.

Marfaing, O., Guingo, M., Lavieville, J., Mimouni, S., Baglietto, E., Lubchenko, N., Magolan, B., Sugrue, R., and Nadiga, B. T. (2017). Comparison and uncertainty quantification of two-fluid models for bubbly flows with NEPTUNE_CFD and STAR-CCM+. *Nuclear Engineering and Design (preprint)*.

Nadiga, B., Baglietto, E., and Stephens, J. (2016). Hydrodynamic closure evaluation in multiphase flow using star-ccm+ (l3 milestone thm.cls.p13.01). *CASL Report*.

Stuhmiller, J. (1977). The influence of interfacial pressure forces on the character of two-phase flow model equations. *International Journal of Multiphase Flow*, 3(6):551–560.

User-Guide (2016). Star-ccm+ version 11.02. *CD-adapco-2016*.