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Dynamic Droplet Sizes for Drift Fluxes

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OVERVIEW

There are many two-fluid mixtures of practical interest. For example, mixtures of air and water or oil and water occur frequently in environmental and industrial processes. The existing modeling capability in ***FLOW-3D*** for mixtures of two fluids is the *DRIFT* routine that computes the relative motion of the two components arising from buoyancy and viscous forces. This model works quite well for many situations because of its simplicity and robustness.

There are two types of two-component flows. One is a mixture of two fluids having different densities, but no sharp two-fluid interface. The other type is a single fluid, which may have a free surface, but with a variable density arising from the mixture of two incompressible components (e.g., air entrainment in water).

In the *DRIFT* model one component is typically dispersed in the other component. Usually, it is assumed that the component having the smallest volume fraction is the one that is dispersed in the sense of being separated into many disjoint pieces that are surrounded by the other, continuous, component. It is often convenient to think of dispersal as consisting of droplets or bubbles. This model, however useful, requires the user to specify the average size of the dispersed material elements so that forces driving any relative motion can be computed.

Specifying a dispersal size has its limitations because it is often not something that is known. Furthermore, sizes can vary in both space and time, for instance, in a mixing vessel containing an impeller it is likely that sizes are smaller near the impeller and may be further decreasing with continued mixing. An exception to this is a dispersed component of solid particles, whose size is fixed in space and time and must be specified by the user.

In this report a new model is described that dyn*amically* computes dispersed fluid droplet sizes within the *DRIFT* routine. The model is based on simple mechanisms for the breakup and coalescence of dispersed material. Users may initialize this model and expect to have a simulation involving the relative motion of components in a mixture that is as good as or better than a simulation with only a fixed size. The greatest feature of the new model is that it produces sizes that vary in both space and time as they adjust to the details of the flow.

BASIS OF DYNAMIC MODEL

A new scalar variable, *dfdiam*, is used to record the averaged dispersed element size (i.e., diameter of a volume-equivalent-sphere) in each computational grid element. This quantity is then used in the *DRIFT* routine to compute the drift-flux velocities. At the end of the *DRIFT* routine the average particle diameter in each grid cell is then updated. Updating is done by using the particle diameter and the volume of dispersed material in each grid element to compute the number of particles in each element. This number changes by breakup and coalescence processes arising from the dynamics of the flow.

Experience shows that drops and bubbles can be pulled apart or broken into two or more pieces by a strong enough shear applied across the element. Typically the resistance to being pulled apart is surface tension. In the case of a strong velocity shear the non-dimensional number characterizing the relative strengths of shear and surface tension is the Weber number,

$$W_e = \frac{\rho_a U_r^2 \cdot dfdiam}{8\sigma}$$

Here ρ_a is the volume averaged density of the mixture fluid surrounding a dispersed element, σ is surface tension and U_r is an effective relative velocity.

Experiments show that a critical value for breakup occurs at about a Weber number (as defined above) of 1.6 [1]. Different experiments show small variations in this value, but 1.6 would seem to be a reasonable choice (an input variable *webcrit* can be used to change this value). It should also be remarked that some authors use a different expression for the Weber number, for example, they may make a different choice for the length parameter or they prefer to omit ½ from the dynamic pressure compared to the surface tension pressure.

In highly viscous flows spherical elements may be pulled apart by viscous shear stresses as opposed to dynamic shears, in which case the relative strengths of shear and surface tension is better characterized by the capillary number

$$C_\sigma = \frac{\mu_a U_{df} + \mu_{turb} dfdiam \cdot e}{2\sigma},$$

where μ_a is the volume averaged molecular viscosity of the mixture fluid surrounding the dispersed element and μ_{turb} is turbulent viscosity. For this work, a critical value for breakup has been estimated to be about 1.0 [1], which can be changed using the input variable *capcrit*.

A decrease in the number of dispersed particles may occur because of coalescence caused by collisions. A simple collision model has been formulated in terms of the number of encounters expected when a particle moves with respect to its neighbors. Putting the breakup and coalescence processes together then yields a rate equation for particle number per unit fluid volume.

The update of the particle number is done at the end of the *DRIFT* routine. Finally, the new particle number in each grid element is converted back into an average particle diameter *dfdiam* in that element ready for the next computational cycle.

Regions of pure fluid, i.e., regions containing no mixture, are given a zero particle size indicating that size has no meaning where there is no dispersed material.

EXAMPLE SIMULATIONS

Finding good data with which to validate the dynamic droplet model is difficult. There are numerous experiments about the mixing of two fluids, but they rarely include measurements of the sizes, or size distributions, of the dispersed material. In the following are several example cases in which some data has been found or results are at least what would be expected.

Oil-Water Separation

An example illustrating the *DRIFT* model addresses the separation of an oil and water mixture. Initially the oil and water are mixed in a blender for some time; the size of the dispersed phase (oil) droplets that result from this mixing is not known. This mixture is then poured into a vertical cylinder of height 0.915m and allowed to separate in which the lighter oil moves to the top and the water to the bottom. There is no mean flow velocity of the mixture in the cylinder and therefore no shear stresses and no turbulence that could change the size of dispersed particles. Thus, for this example, the dynamic droplet model should have no influence on the separation, but simulations were run to make sure of this. A drop size must be specified at the start of the simulation (representing the initial blender preparation). In this case, the drop diameter was guessed to be 0.0012m, a value that had been found to give good results in comparison with experiments when simulated with the constant size option.

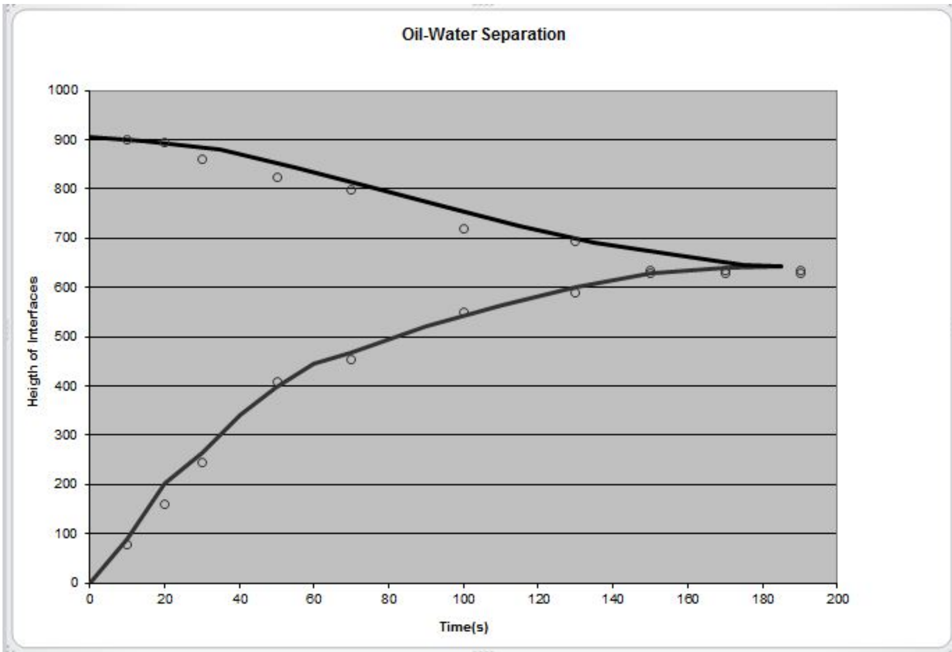

Figure 1. History of oil and water separation interfaces (oil at top, water at bottom). New model does not change droplet sizes because there are no mechanisms for coalescence or breakup. Solid lines are experimental values and circles are simulation results.

Using the dynamic drop model, the resulting simulation does reproduce the constant drop size results. There are no breakup or coalescence processes and the computed size remains at its initial size in the mixed region, but has been set to zero at the top and bottom regions where pure oil and water have formed. The height histories of the top and bottom interfaces separating pure fluid from the mixture are shown in Fig.1.

This example is important, because it emphasizes that some problems require the user to supply an initial size when there are no shear or turbulent effects operating that could sort out realistic sizes. For this reason, it has been found necessary to always initialize the dispersed element size beforehand. The dynamic droplet model, if activated, will quickly adjust the initial value if breakup and/or coalescence forces are operating.

Mixing Tank

A second example that illustrates the basic operation of the dynamic droplet model is a mixing tank driven by a single impeller. This tank and impeller setup has been a standard test case for ***FLOW-3D*** and has previously been shown to give good agreement with measured velocity distributions for a uniform density fluid having no free surface. In this case the fluid is treated as a variable density, single-fluid model consisting of a mixture of two fluids of density 1.0 and 0.837 gm/cc (water and oil). Initially the lower half of the tank is water and oil resides in the upper half. Surface tension at the oil/water interface is 52.4dyne/cm and the viscosities of oil and water are 0.0126 and 0.01poise.

The tank is cylindrical having a radius of 7.3cm and height of 14.6cm. The impeller, a Ruston type, is located at the midpoint of the central axis and is modeled using the fan/impeller feature in ***FLOW-3D***. The radius of the blades is 2.44cm and their vertical extent is 0.8cm. The blades are rotating at ten revolutions per second and are tilted to force a downward axial flow.

In the simulation of this problem a fixed diameter size is used for the initial dispersed fluid at 0.5cm. Using the new dynamic droplet model the size distribution, at steady conditions, Figs.2-3, ranges from diameters of 0.0cm to 3.19cm, with an average above 1.5cm. The average diameter is larger than the mesh cell sizes. Using such large sizes in the DRIFT model is somewhat questionable, but has not produced anything unrealistic.

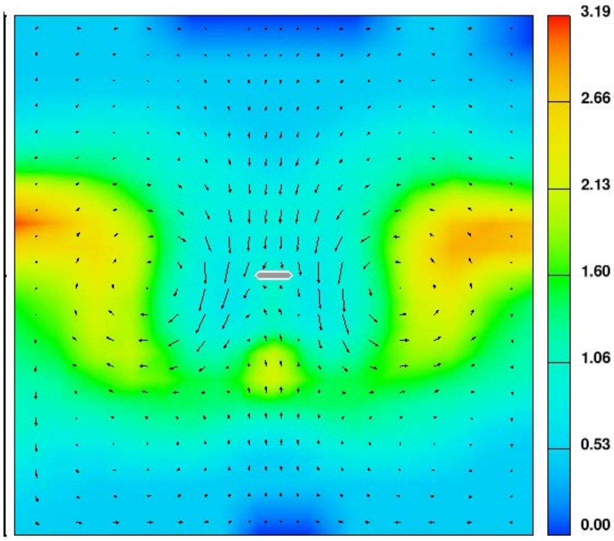

Figure 2. Size distribution in middle vertical x-z slice.

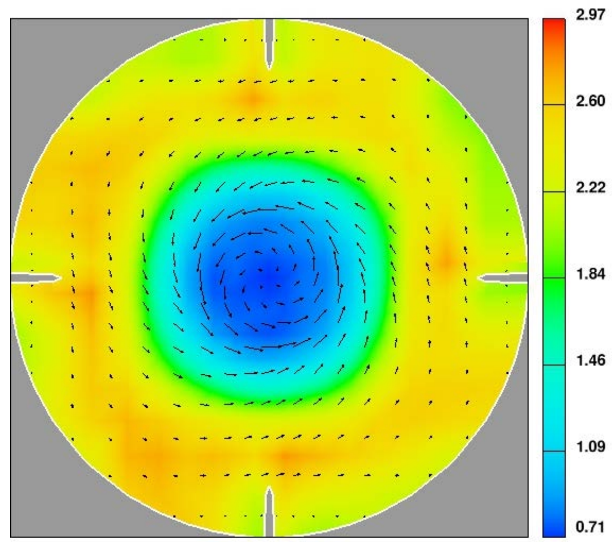

Figure 3. Size distribution in middle horizontal slice.

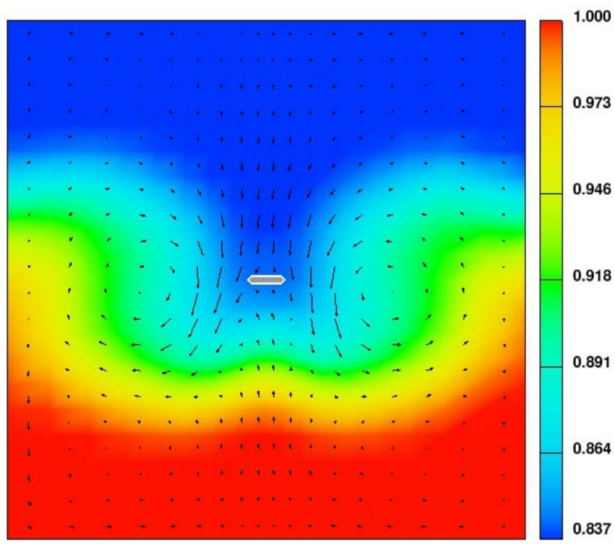

Figure 4. Density in middle vertical slice.

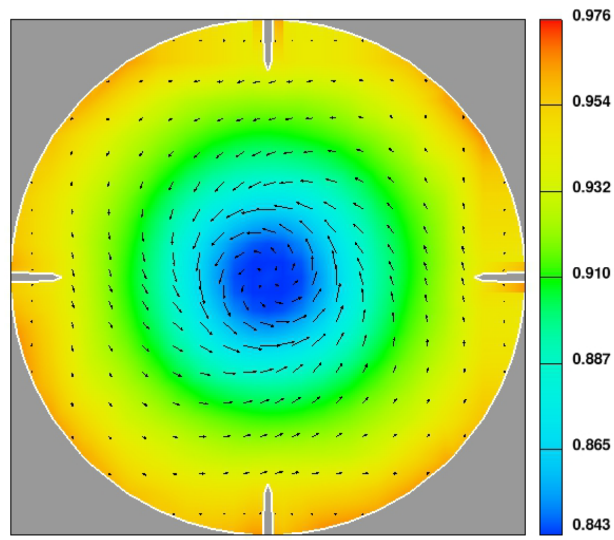

Figure 5. Density in middle horizontal slice.

Figures 4 and 5, show the mixture density at steady state where it can be seen in Fig.4 that there is bottom layer of nearly pure water and a top layer of pure, or nearly pure oil confirming the lack of mixing of the two fluids. Only the central region exhibits some mixing. In Fig.5 the density is low in the center where flow is descending from the lower density region above and larger near the side wall where is moving upward from the denser lower region. Apparently the location, size and spin rate of the impeller is not sufficient to mix the two fluids, except in the near vicinity of the blades.

Referring back to Fig.2 it is seen that the size of drops has been set to zero in the top and bottom regions of almost unmixed fluid. Using a size of zero in unmixed regions is done to avoid confusion that might arise from having odd sizes in such regions where there is no mixing of fluids, i.e., regions where droplet size would have no meaning.

These results look reasonable and consistent with the limited mixing produced by the impeller. However, there exist no actual data for this example that can be used to confirm the droplet sizes predicted.

Spillway Air Entrainment

The entrapment of air in water flowing down a sloped spillway is a good example of a one-fluid, variable density flow consisting of a mixture of water and air (i.e., a gas/liquid mixture). The shear of the water on the bottom of the spillway generates turbulence that reaches the free surface of the water and entrains air. Simulating this is best done with the ***FLOW-3D*** advanced air-entrainment model that includes buoyancy and bulking of the water-air mixture. Earlier simulations of a spillway flow using a specified bubble size for the dispersed air phase are documented in [3]. Because this flow is strongly affected by shear and turbulence it is an obvious case where the dynamic droplet model should be used.

The test case selected was one in which data for entrained air bubble sizes were actually reported. An experimental laboratory study [4] was conducted in which water 0.05m deep is flowing down a chute tilted 5.71° with respect to the horizontal (tilting is modeled using a tilted gravity vector). The chute is 14m long and 0.5m wide. Water at the inlet to the chute was 0.05m deep and the inlet flow rate was 0.1755 m^3/s. This flow corresponds to a Froude number of 10.03 and contained 17.76% air and 10% turbulence. Air is also entrained at the surface of the flow and adds volume (bulking) to the mixture, as can be seen in Fig.6, which shows only the first meter of the chute. It can also be seen that the buoyant rise of bubbles has reduced the inlet air concentration at the bottom of the chute at the right end. After about one meter from the inlet the flow appears nearly uniform in depth and distribution of air and bubble sizes.

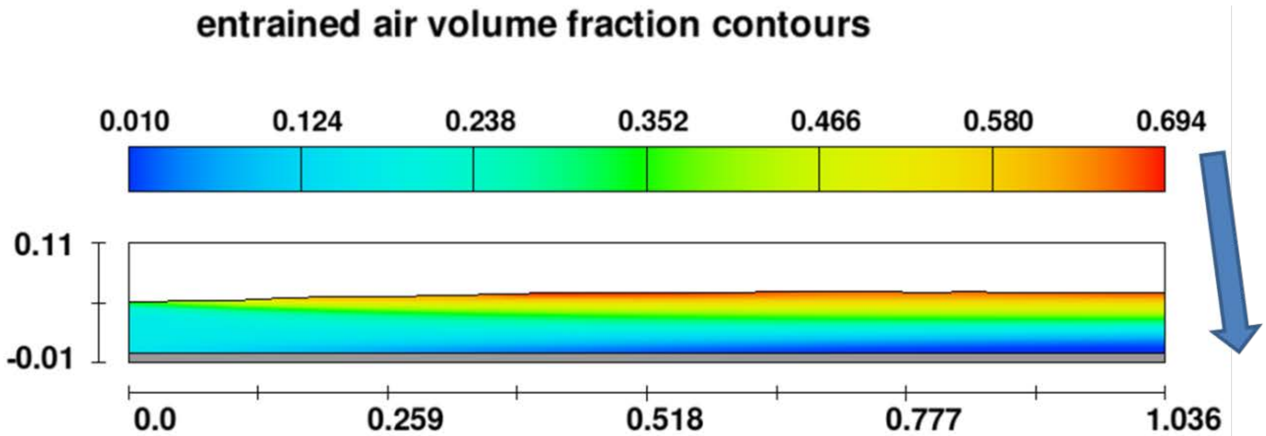

Figure 6. Air volume bulking up fluid in first meter down chute.

A simulation was performed for one symmetric half of the chute using the dynamic drop model together with drift and bulking for the entrained air. An initial input bubble diameter of 0.001m was used and the air was also assumed to always be the dispersed phase regardless of its volume fraction. In the experiment the nominal free surface of the flow was assumed to be at the location where the concentration of the air is 90% (or 10% water). In the simulation this condition is imposed by using the air escape mechanism and limiting the minimum water volume fraction to be 0.1. The 90% air assumption for defining the surface is a common one for spillway studies, and measurement have shown that the mass and momentum of water flowing down chute above this level is negligible.

The computed volume fraction of air in a cross section of the symmetric half of the chute, at the end of the chute where the flow is nearly steady and uniform with respect to the flow direction, is shown in Fig.7a along with the distribution of bubble size, Fig.7b, in the same cross section. A small disturbance exists at the outside wall, which has some time dependence. This is associated with what the experimentalists observed as roll waves emanating from the sides of the chute.

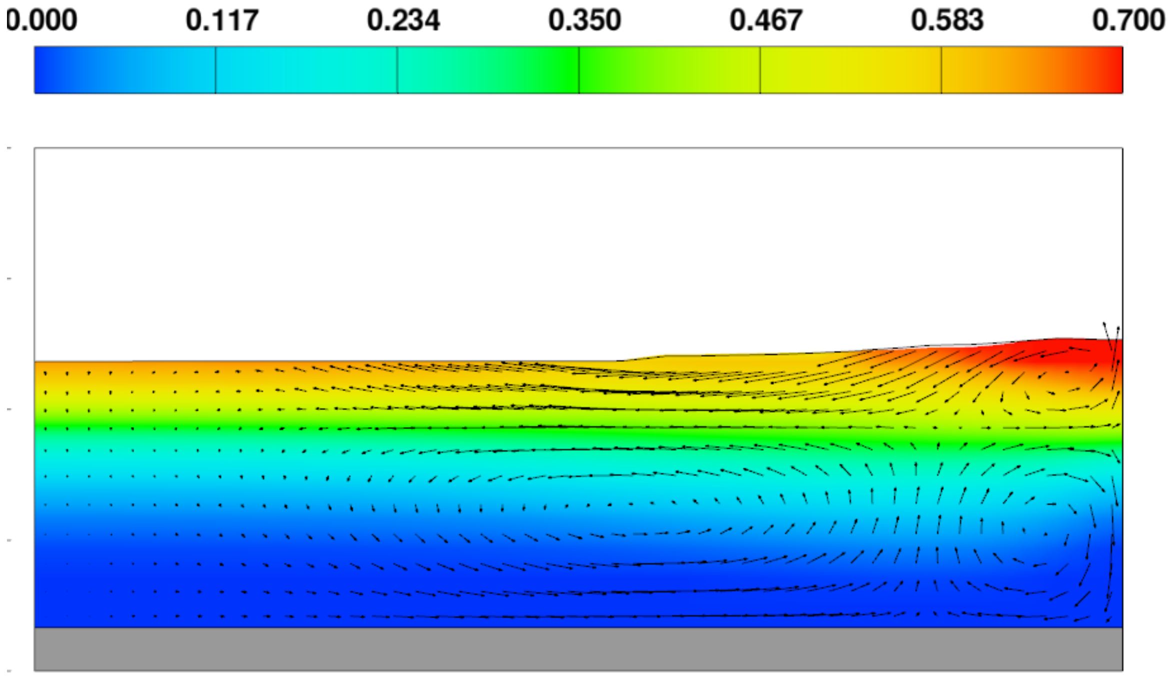

Figure 7a. Symmetric half of air concentration at end of chute.

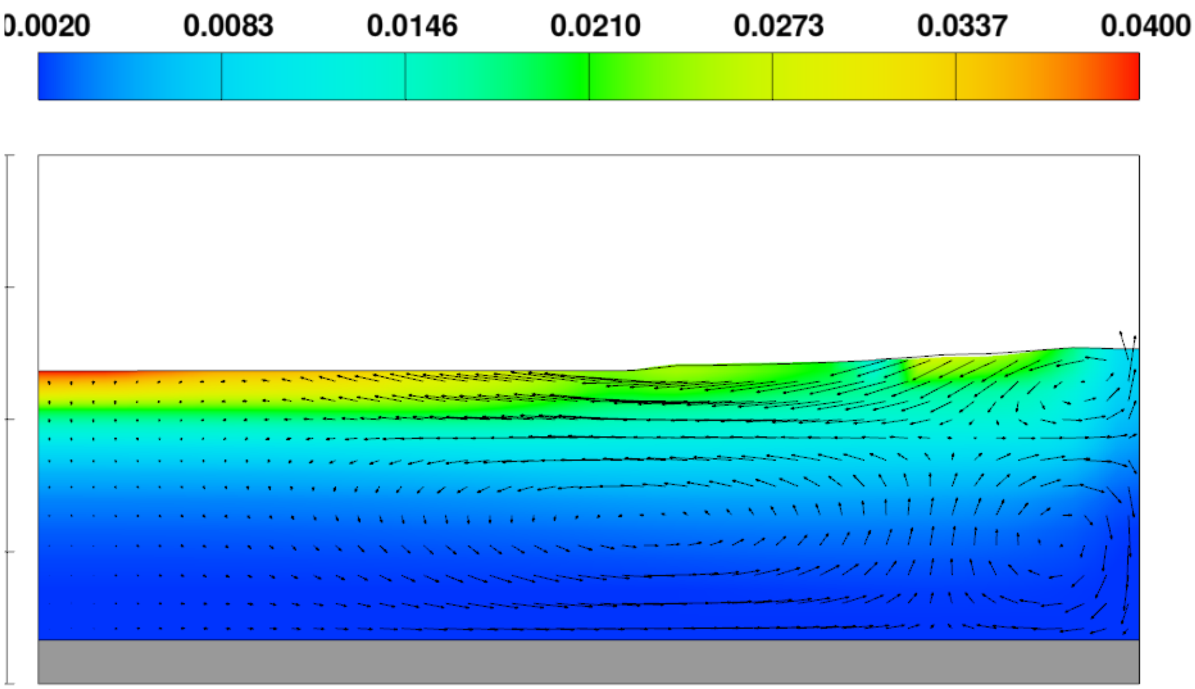

Figure 7b. Bubble diameter distribution at the end of chute (m).

The computed depth of flow (to the 90% air level) is 0.061m. Depth data reported in Ref.4 is not consistent or clear, but in Fig4.6 of Ref.4 the 90% height is 0.062m if heights have been normalized by the value 0.044m indicated in the plot. The experiments are also reported to have an average air content at the end of the chute of about 16.7%, whereas the simulation has a value of roughly 20%.

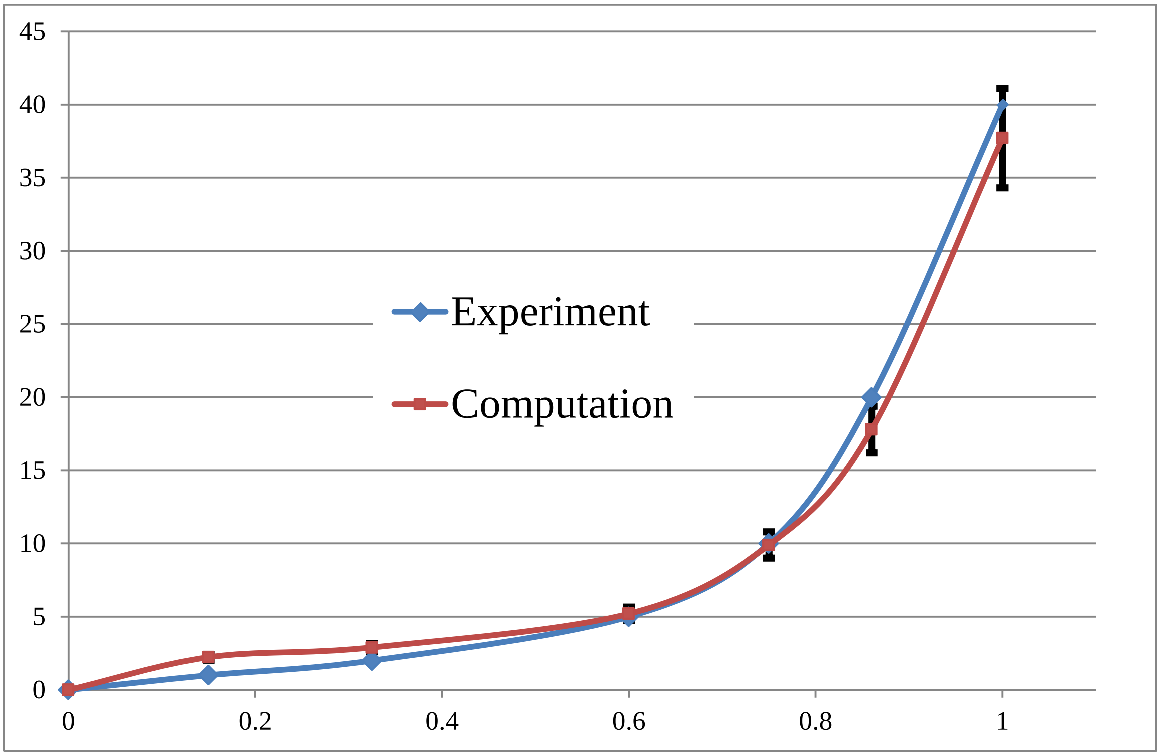

Figure 8. Computed bubble diameters from floor of chute to top of water in comparison with experimental data at the end of the chute. Errors bars on the computational results indicate variations with time since the solution is only quasi-steady.

Finally, a comparison of simulation results with experimental data for bubble diameters versus depth, at the midpoint of the chute is shown in Fig.8. Sizes vary from about 2mm to 4cm, a considerable range. The agreement of the simulated sizes with data is quite remarkable and can be considered a good, first, validation for the new model involving actual data on the size of elements of a dispersed fluid within a second fluid.

Summary

The drift-flux model has been extended with the addition of a simple model for predicting the size of dispersed material in liquid-liquid and liquid-gas mixtures. The extension, referred to as the Dynamic Drop model, computes breakup and coalescence of droplets caused by shear and turbulent flow processes. This model provides a size for dispersed material that is both time and space dependent that is far superior to the constant size previous required in the drift model.

Several examples have been described to illustrate what can be expected from the new model. It has also been noted that good data about the sizes of dispersed material particles are difficult to find. One study of chute flow has been successfully simulated, but more validation tests should be conducted.

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4. Kramer, K., *Development of Aerated Chute Flow*, Technischen Hochschule, Zürich (2004).