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A SURFACE TENSION MODEL UPDATE

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PURPOSE AND BACKGROUND

The modeling of surface tension forces is computationally difficult because it requires the evaluation of surface curvatures, i.e., second derivatives of the surface location. This is particularly true in ***FLOW-3D***® since it uses a regular rectangular grid that does not conform to surface shapes. Although this simple grid structure makes it more difficult to evaluate surface slopes and curvatures, it is this feature that also gives the strength needed to simulate coalescence and breakup of fluid blobs.

Evaluation of surface slope and curvature in ***FLOW-3D***® is done by determining which coordinate direction is closest to the outward normal vector to the surface. Then fluid in a 3 by 3 by 3 set of grid cells surrounding a given cell is summed up in the cell columns parallel to the normal. This, in effect, gives a discrete representation of the surface height in nine (3x3) columns, which can be used to compute slopes and curvatures.

In most cases this procedure works quite well, but when normal directions in the grid are near 45° the surface may be too steep for this procedure to work accurately. A consequence of this loss of accuracy is the introduction of spurious pressures or perturbations that sometimes generate undesirable capillary waves (i.e., kinetic energy noise). Occasionally, these perturbations can even destroy a computation.

A summary of the original surface tension model was given in Technical Note TN6, "Surface Tension Validation Tests," (1987). Since that Note there have been a number of major improvements:

1. Wall adhesion sensitive to slope of wall,
2. Static contact angle as an obstacle property,
3. Two-fluid interfacial surface tension,
4. Thermocapillary (i.e., tangential) surface forces (see TN47).

In this Technical Note we document another improvement that has been made. In particular, we have improved the accuracy of the column summation technique for the computation of surface curvatures. As the following examples will show, this improvement is quite dramatic in many cases where the earlier model experienced substantial difficulties.

SAMPLE TEST CASES

The following examples are simple test cases that demonstrate the effectiveness of the revised surface tension model. This model is available in program Versions 7.5.2 and above.

Axisymmetric Drop at Equilibrium

A spherical drop is initialized in cylindrical coordinates. Although the drop should remain at rest, there will be some variation in the initial surface tension pressures because of numerical approximations. These pressure variations introduce perturbations on the surface of the drop, but if the computational method is sufficiently robust they should remain bounded and the drop should maintain a nearly spherical shape.

Figure 1 shows the cross section of a drop of water having a diameter of 0.3 cm after 1.0s of computational time (i.e., after tens-of-thousands of time steps). The initial outline of the drop is also shown to emphasize how little the drop has deformed. Clearly, the drop deviates very little from its initial spherical state. Fluctuations in average kinetic energy remain bounded, but do not damp out very quickly because of the relatively low viscosity.

In the original surface tension model the drop suffers very large deformations and hits the outer boundaries of the grid.

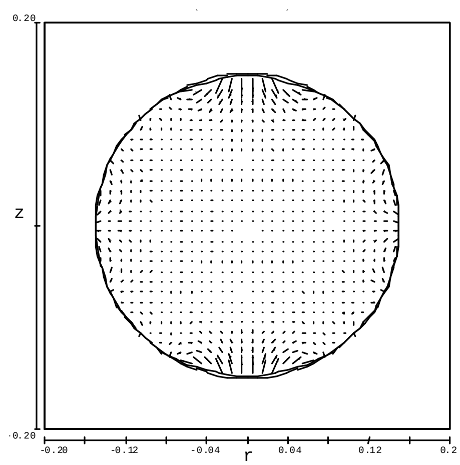

Figure 1. Axisymmetric drop after 100,000 time steps compared with initial drop shape.

Three-Dimensional Drop at Equilibrium

A repeat of the above computation was undertaken using a three-dimensional rectangular Cartesian grid. Symmetry boundary conditions were used to restrict the simulation to a single quadrant (i.e., 1/8 of the full drop).

In this case the surface tension pressures are reasonably well predicted, but a bit of liquid squirts out from the drop's surface at the 45° location. This squirting is partly caused by small advection errors in the fluid fraction. At the 45° location it is very difficult to compute the movement of small amounts of fluid in and out of the corners of grid cells.

Increasing the viscosity by a factor of 10 helps to slow down the motion generated by the initial pressure variations. Figure 2 shows a slice through one of the planes of symmetry after a time interval of 0.05s (about 5100 time steps) with the initial profile of the drop over laid for comparison.

Although the escaping bits of liquid are undesirable, this result is still much improved over the results produced by the previous model in which the drop rapidly shakes itself apart.

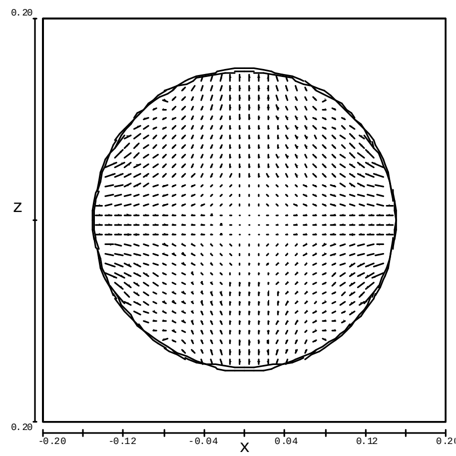

Figure 2. Three-dimensional drop after 5100 time steps compared with initial drop shape.

Spherically Capped Column of Liquid

Ink jets often involve long columns of ink that eventually contract into droplets. A test of jet contraction can be made by constructing an initial liquid column that is longer than its diameter. For illustration we have given one end of a cylinder a spherical shape and made the other end a plane of symmetry. The fluid is water and the initial diameter of the cylinder is 12 microns (12.0e-4 cm).

Two simulations have been performed. One was an axisymmetric case and the other a three-dimensional model for one 90° quadrant.

The original surface tension model was not able to produce results for these two cases that looked similar. Results from the original axisymmetric case are included in Fig.3 in the left frame.

The improved model has no difficulty with this comparison even though relatively coarse grids were used (i.e., 14x40 and 14x14x40). The middle frame of Fig.3 shows the liquid surface at four times (0.0, 4.0, 8.0, and 12.0 μs) for the axisymmetric case. The right frame in Fig.3 shows

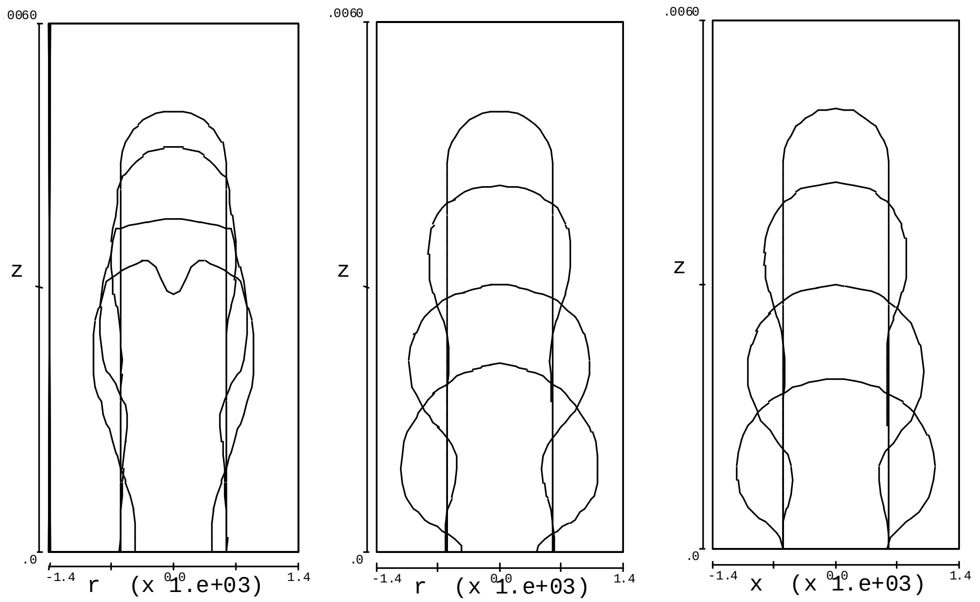

Figure 3. Comparisons between simulations for the retraction of a column of liquid. Surface shapes are shown at times of 0.0, 4.0, 8.0, and 12.0 μs. The original model's axisymmetric results are at left, the new model's axisymmetric results are in the middle and its 3D results are to the right.

the corresponding results for the three-dimensional simulation using the new model. There is excellent agreement between the two new cases. The only significant difference observed in those two simulations is at the bottom symmetry plane at the last time shown.

The problem with the original calculation is that some locally low values of surface-tension pressure are computed near the 45° location, which produce the corner-like shape obvious at 8.0μs and slows down the overall retraction rate of the column.

It is rather obvious that the new model is producing significantly better results. Not only are the axisymmetric and three-dimensional cases nearly identical, they both compute without difficulty and exhibit a realistically smooth appearance.

SUMMARY

An extension has been made to the algorithms used for evaluating surface curvatures. As this Technical Note demonstrates, the extension greatly improves the performance of the surface tension model used in ***FLOW-3D***®. Not every problem will run perfectly, but the improvement in computability offered by the new model is dramatic for a number of situations that were previously difficult to simulate.