

SURFACE TENSION MODELING

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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*¹ since it uses a 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 fluids.

A new update to the surface tension model introduced in *FLOW-3D*, Version 11, greatly improves the accuracy of the model with regard to the computation of curvatures as well as improving the application of wall adhesion forces. Additionally, the new model fully integrates thermocapillary forces, i.e., tangential surface forces, into the basic model without the need for a separate model routine.

Briefly, the evaluation of surface slope and curvature in *FLOW-3D* is done by first determining for each computational cell that contains a surface the coordinate direction that is closest to the outward normal vector to the surface. Following this, cell columns containing 3 cells that are associated with the surface cell and its four principal neighbors (i.e., those located perpendicular to the principal surface normal) have their fluid fraction values summed up in the direction of the normal. This effectively gives a discrete representation of the surface heights in five columns surrounding the surface cell, which can then be used to compute slopes and curvatures at the surface. These heights are also used to compute the surface normal and area for the cell.

To compute the forces of adhesion between a fluid surface and a solid it is necessary to determine the location and extent of the contact line where the fluid and solid surfaces intersect. In the newly updated model this determination is done separately at each side of a surface cell, i.e., those sides whose normals are perpendicular to the principal surface-normal direction. Associated with each element side, the orientation of the solid surface and its specified contact angle are evaluated and used to compute the proper adhesion force components. These forces replace the fluid-to-fluid values that may have been computed in the basic surface tension force computation, or at least those forces for the portion of the side area that is blocked by the solid.

There are a few special cases that must also be considered. For instance, the obstacle in the surface cell may lie entirely below or above the fluid surface in which case there would be no contact line. Also, at a mesh boundary that is a plane of symmetry there is an apparent area

¹ *FLOW-3D* is a registered trademark in the US and other countries.

blockage but there is no physical wall surface. In such cases the contact angle is set to 90° corresponding to symmetry conditions.

The new approach described here goes well beyond what was previously done, as it looks in each coordinate direction as well as evaluates the orientation and specific contact angle of every solid surface that might intersect the surface cell. The previous approach was only able to distinguish average solid properties and orientations within a surface cell.

ILLUSTRATIVE TEST CASES

The following examples are simple test cases that demonstrate the effectiveness of the new surface tension model. These examples were chosen mostly from cases where the original method did not work well in order to emphasize the improvements provided by the current update.

Wetting of a 2D Cylindrical Tank in Zero Gravity

This example tests the ability of the model with a zero contact angle to fully wet a cylindrical surface in the absence of gravity. A cylindrical tank has a radius of 5.0cm and is initially half filled with fluid of density of 1.0g/cc, viscosity 0.01gm/cm/s and surface tension 100.0dynes/cm. Figure 1A shows the computed results at times 0.0, 0.5, 1.0 and 2.0s for the original (not updated) surface tension model. The wetting points of the surface appear pinned at locations near the top of the cylinder, even though a zero contact angle should be able to pull the fluid surface all the way to the top. At later times this simulation eventually does wet the entire boundary, but the development is not realistic.

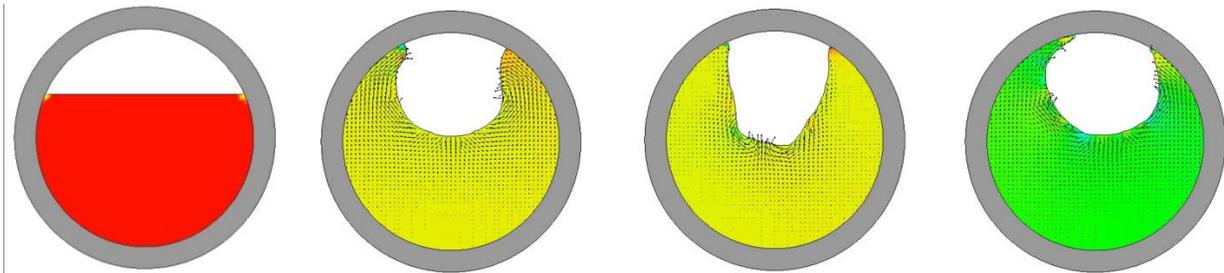


Figure 1A. Simulation using old model of 2D cylindrical tank in zero gravity at times 0.0, 0.5, 1.0 and 2.0s. Color indicates pressure, although the scale is different in each frame.

A repeat of this problem using the updated model is shown in Fig. 1B where it is seen that the surface is now fully wetted and a bubble has been detached from the wall of the cylinder by 1.0s.

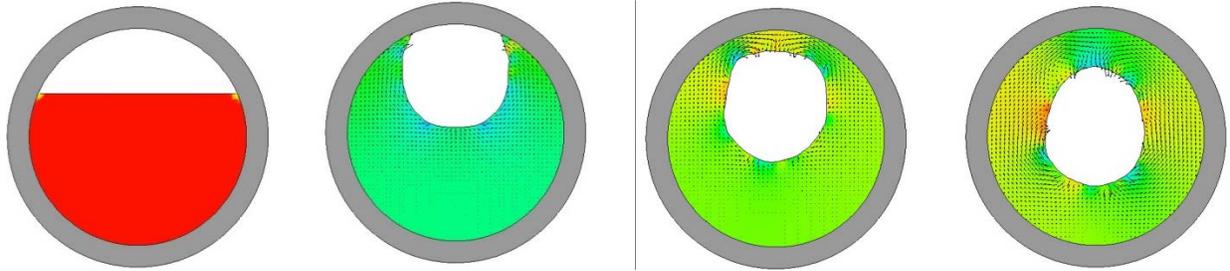


Figure 1B. Simulation using updated model of 2D cylindrical tank in zero gravity at times 0.0, 0.5, 1.0 and 2.0s. Note continuous and symmetrical wetting of surface. Color indicates pressure, but with a different scale in each frame.

Downward Moving Spherical Drops

Another example to illustrate the improvements made in the surface tension model involves two spherical drops, side by side, that are given an initial downward velocity of 20cm/s. The drops have a radius of 0.085cm. One drop is iron with density 7.0 and viscosity 0.05, while the other drop is aluminum with density 2.7 and viscosity 0.013. Both drops have the same surface tension coefficient of 1872.0.

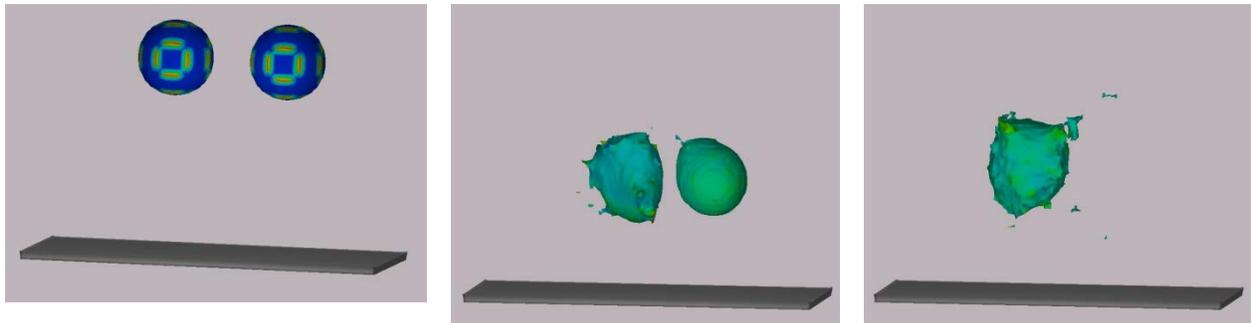


Figure 2A. Moving Drops computed with previous model at times 0.0, 0.01 and .02s. Color indicates pressure.

Figure 2A shows the simulation results for the moving drops that were obtained with the original surface tension model. The times shown are 0.0, 0.01 and 0.02s. By 0.01s the drops have undergone significant distortion and by 0.02s have merged, with some shedding of small droplets.

Figure 2B shows the simulation results obtained with the updated model at times 0.0, 0.01 and 0.2s. The drops remain nicely spherical as they move down through the computational grid and they continue to move with almost the same velocities. This last condition is not assured because the computed surface tension pressures, applied over the entire surface of a drop, are not guaranteed to produce a net zero force as would be expected physically. The difference in appearance of the drops in the last frame, however, is the result of the left-hand drop striking the plate slightly before the right-hand drop.

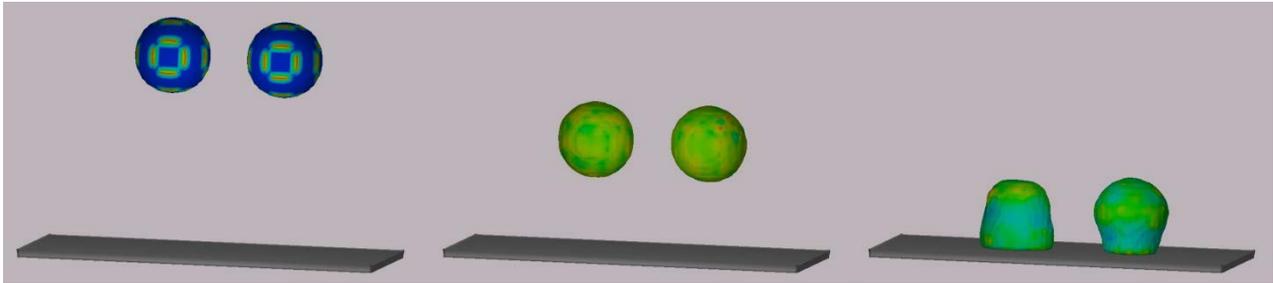


Figure 2B. Drops computed with updated model at times 0.0, 0.01 and 0.02s. Color indicates pressure.

A cleaning up of small fluid bits was used in all the drop simulations by setting $f_{clean}=0.05$. The updated surface tension model is performing considerably better than its predecessor.

Capillary Rise in a Square Channel Rotated 45°

Capillary rise is an often encountered result of surface tension forces. For this test example the capillary rise is computed for a square channel that is rotated 45° in the horizontal plane of the computational grid. The symmetry of the problem requires only one quarter of the channel to be simulated, which is used here as a simplification. The full channel has a diagonal width of 1.0cm corresponding to a side edge length of 0.707cm. The fluid is being pulled up the channel against gravity ($g_z=-980\text{cm/s}^2$), with density 1.0gm/cc, viscosity 0.1gm/cm/s and surface tension 70dynes/cm. The wall contact angle in the channel is 30°. A rather coarse grid of 21x21x40 cells was used for the simulation.

A simulation obtained with the original surface tension model did not run very well initially because small bits of fluid were shed with some very large velocities that kept the time-step exceedingly small. To alleviate this problem a cleanup option was activated using $f_{clean}=0.05$, and this allowed the simulation to proceed efficiently. The results are shown in the left frame of Fig. 3. They are not very clean and still have many small pieces, not shown in the plot, above the surface. The amount of fluid raised is about 12.1% below the expected theoretical value.

For comparison, the simulation results from the updated model (without the f_{clean} option) are shown in the right frame of Fig. 3. Here we see a much smoother surface profile and there are no small bits of fluid lying above the surface. In addition the amount of fluid pulled up is only 3.8% below the theoretical value. The computed contact angle at the wall in the symmetry planes is the 30° specified, as would be expected.

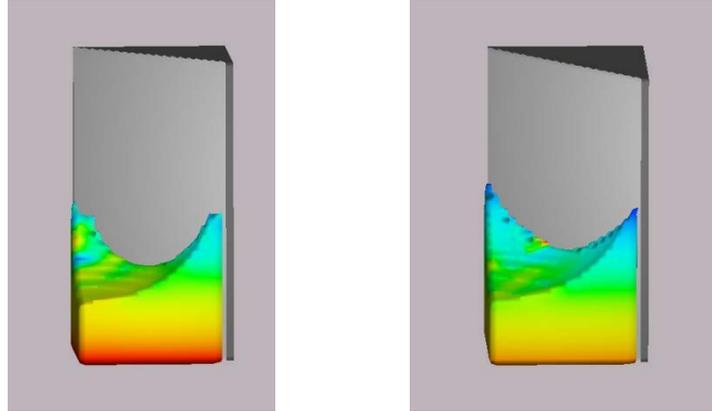


Figure 3. Simulation results for capillary rise in a square channel rotated 45° . Previous model on left and updated model on right. Color indicates pressure.

Bubble within a Liquid Drop

An interesting surface tension example that also employs adiabatic gas bubbles is that of a small liquid droplet resting on a horizontal surface and containing a small gas bubble in its interior. Gravitational buoyancy causes the bubble to rise to the surface of the liquid drop and pop through. Surface tension forces are acting on the droplet surface as well as the surface of the interior bubble. In this example the initial radius of the droplet is 0.07765cm while that of the bubble is 0.0075cm. The liquid is water, gravity is downwards and the ratio of specific heats of the air in the bubble is 1.4. The contact angle of the drop on the base plate is 75° .

Figure 4 shows four snapshots of the axisymmetric simulation at times 0.0, 0.0018, 0.0021 and 0.0040s. These results were obtained using the new surface tension model; the previous model was not able to do this problem at all because pressure fluctuations were too large to resolve the net buoyancy of the bubble.

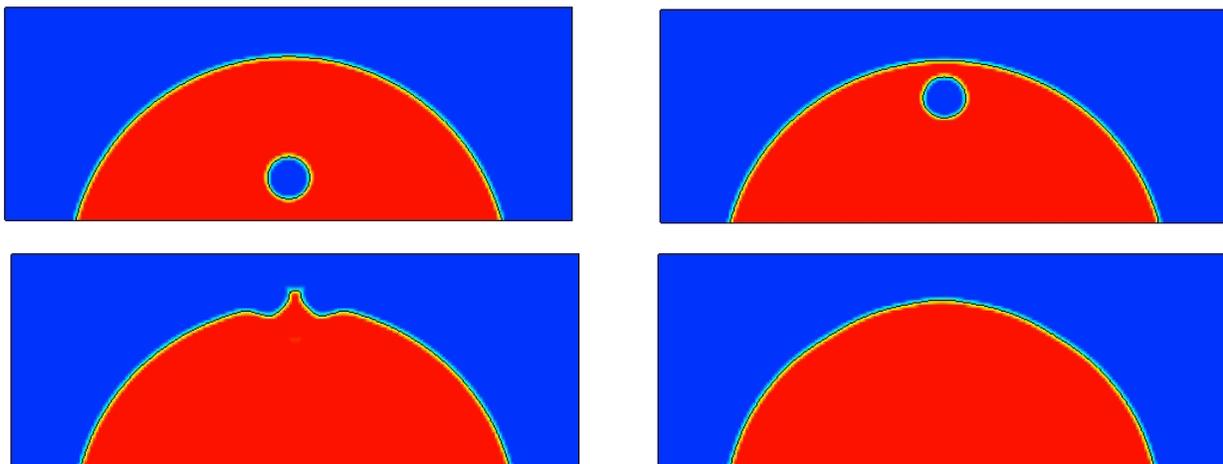


Figure 4. Bubble in drop on plate. Upper left at $t=0.0$ s; upper right at $t=0.0018$ s; lower left at $t=0.0021$ s and lower right at $t=0.004$ s. Color indicates fluid density.

Wicking into a Porous Medium

A somewhat different example of surface tension involves the wicking of liquid into a porous material. The wick is cylindrical in shape with a diameter of 2mm and length 8mm. Initially the wick is immersed into a pool of water to a depth of 0.5mm. The pool itself is maintained at a depth of 2.5m by boundary conditions at the sides of the computational region. The wick has a porosity of 0.3, a capillary pressure of $1.46 \times 10^4 \text{ dynes/cm}^2$ and a porous media drag coefficient (oadrg) of $1.8 \times 10^6 / \text{cm}^2$. The contact angle of water on the wick's surface is 60° .

Snapshots of the filling history of the wick are shown in Fig. 5 at times of 0.0, 0.5, 1.0 and 1.5s. The wick is not quite 100% filled at the end of the simulation and there appears in the lower-middle of the wick a small region of incomplete wetting of the wick. The liquid volume fraction in this region is, however, above 50%. This region, which develops as the liquid diffuses in from the bottom and sides and traps a small amount of air, represents a very small volume fraction because it is centered on the axis of symmetry. The exterior liquid establishes its 60° contact line on the side of the wick by the first snapshot at $t=0.5\text{s}$ and changes little afterwards.

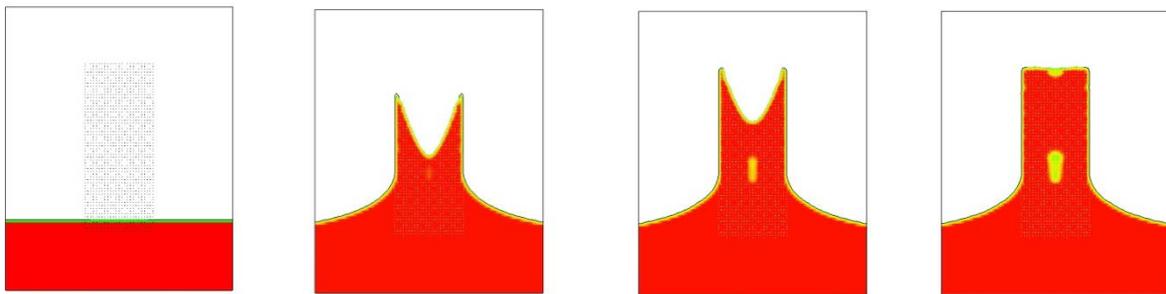


Figure 5. Wicking of water into a cylindrical, 2mm diameter wick. Times are 0.0, 0.5, 1.0 and 1.5s. Color is fluid density.

Marangoni Flow Example

To demonstrate the capability of the new model to describe flows generated by a non-uniform surface tension a simple test case consists of a shallow 8.0cm diameter dish of water of depth 0.75cm and at an initial temperature of 20°C . The water surface is uniformly sprinkled with massless markers. Placed at the center of the circular dish is a cylindrical rod of diameter 0.5cm, which is heated to a temperature of 80°C , and is submerged into the water surface to a depth of 0.05cm. As the water near the hot rod is heated its surface tension is reduced by an amount of $0.1678 \text{ dyne/cm}/^\circ\text{C}$ causing the surface to retract toward the outer rim of the dish.

This problem is similar to what happens in a dish of water when a drop of detergent is placed at the surface center. The surface retracts rapidly to its outer edge. In the case of heating, however, the retraction is much slower because the temperature of the water surface is expanding by relatively slow thermal diffusion, while the detergent is spreading over the surface by molecular attraction and may even reach the limit of a one-molecule thick layer. In any case, the consequences for the surface markers resulting from the change in surface tension, while slower, appear quite similar as shown in Fig. 6.

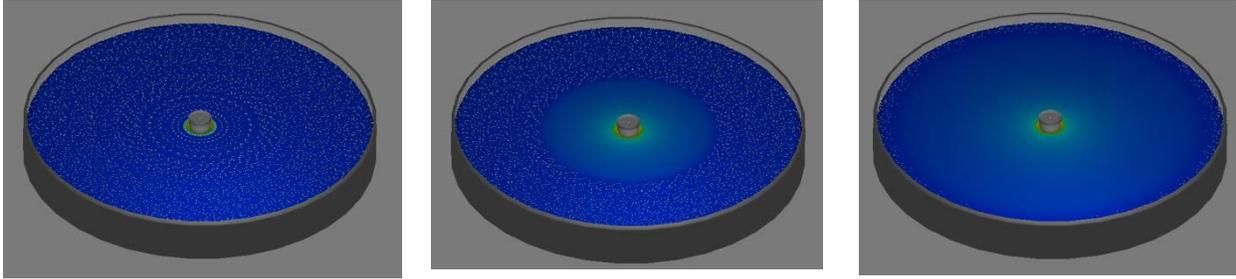


Figure 6. Surface markers retracting to the rim of a dish of water because of a heated rod placed at the center of the dish. Times are 0.05, 1.5 and 3.0s. Color indicates surface temperature.

CONCLUDING REMARKS

A new model for surface tension has been developed that improves upon many features of the previous model in *FLOW-3D*. This model is a synthesis of the old model and the model for tangential forces (Marangoni forces) plus a new approach for wall adhesion forces. Together this synthesis offers a more accurate and robust model, as shown by the examples described in this document.