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Surface Tension Validation – Simple Test Problems

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Overview

Flow problems involving surface tension forces arise in many applications such as microfluidics and liquid fuel behavior in space craft. The ***FLOW-3D*** program has an advanced surface tension model that includes complex geometric, wall adhesion and variable surface tension coefficient capabilities. This document describes a variety of simple problems that have been simulated for which there are simple analytic solutions for comparison. These test cases provide a basic level of validation for the computational model.

Case 1: A Spherical Drop at Rest

A spherical drop of liquid water is considered having radius 0.001m, surface tension coefficient 0.073kg/s^2 and dynamic viscosity of 0.1kg/m/s (100 times water). An increased viscosity relative to water was used to quickly damp residual capillary waves, but does not affect the computed pressure of the drop. Theory, due to Laplace, predicts a pressure p=2sigma/radius, which is p=146N/m^2. A simulation using a uniform grid of cubical cells of edge length 0.0001m results in a computed pressure of 149.72N/m^2, or 2.6% above the theoretical value. Figure 1 shows a cross section and the spherical surface at t=0.012s (1450 computational cycles). At this time the variation in pressure over the spherical surface is only 0.001N/m^2. The maximum residual velocity is of order 7e-7m/s and decreasing with time.

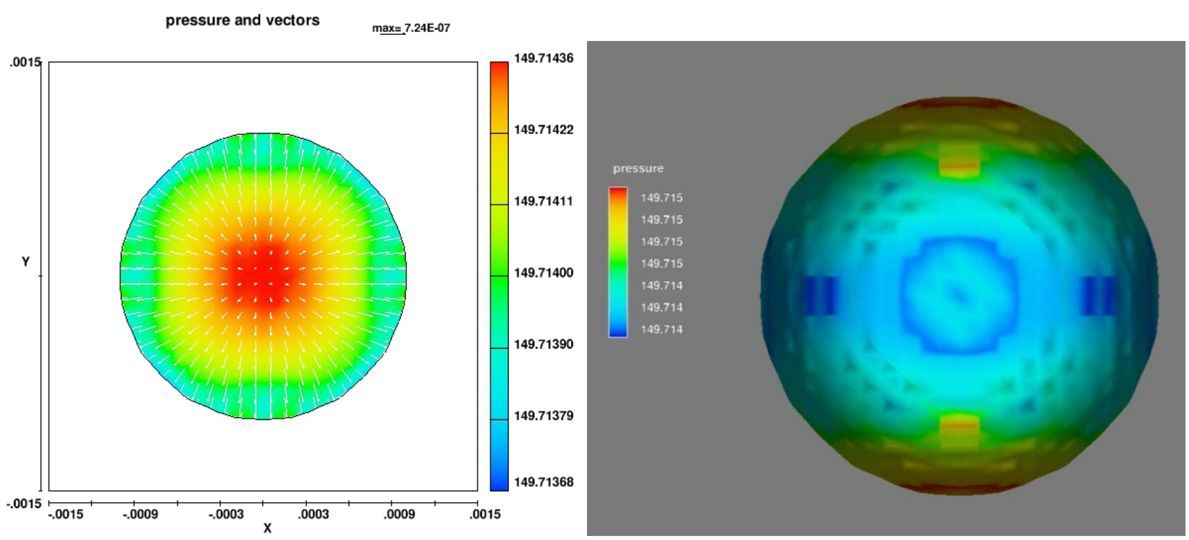

Figure 1. Pressures in cross section of 3D sphere at equilibrium (left) and on full sphere (right).

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A second simulation with double the resolution (i.e, element size 0.00005m) gives a computed drop pressure of p=148.86N/m^2 or 2.0% above theory indicating a small improvement with grid refinement.

Although this is a simple problem its importance for numerical simulation is that the surface has normal directions in all directions and when curvatures are computed with respect to a rectangular grid they are the same over the entire surface.

Case 2: Capillary Rise in a 2D Slot

The second test example considers the rise of liquid in a two-dimensional slot of width 0.1 (roughly cgs units) and thickness w=0.05. The fluid density is ρ=1.0, surface tension coefficient of σ=100, viscosity of μ=0.5 and having a wall contact angle of 30°. A zero pressure is assumed across both the bottom and top of the slot. Wall adhesion is balanced by gravity in the vertical direction of g=1000. Simple theory that balances the upward wall adhesion with the downward weight of fluid pulled up the slot gives a volume of fluid raised to be

$$Vol = \frac{\sigma \cos(30) w}{\rho g}.$$

In the present case the theoretical volume is Vol=0.00433. The equilibrium height of the fluid is about 35 times the width of the slot.

A simulation using a uniform grid of elements of edge length 0.01 (i.e., 10 cells across the slot, although symmetry was used so only half the slot was simulated) resulted in a volume of fluid pulled into the slot of volume 0.0044 or 1.6% above the theoretical value. Figure 2 shows only the top portion of the fluid column after the fluid rise has reached an asymptotic limit.

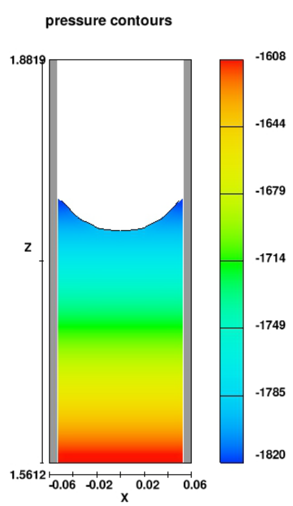

Figure 2. Top portion of fluid pulled up in a two-dimensional slot by capillary action.

Repeating the simulation with 16 cells across the slot gave a volume of fluid raised that was

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2.2% below the theoretical value. This is a little farther from the theoretical value than it was in the coarse mesh simulation, although the change in resolution is not much better than the 10 cell case. For these results a new secular instability treatment was used that is now available (see Appendix) by setting the variable ***ifloss=1*** in the input file.

Case 3: Capillary Rise in a Square Hole Rotated 45° in a Rectangular Grid

Expanding on Case 2 a three dimensional capillary rise problem consisting of a square cross sectioned tube has been simulation. But, to complicate matters a little, the tube is rotated about its long axis by 45° so that its edges intersect the grid elements across element diagonals. As before the pressures applied at the bottom and top of the tube are zero. The edge length of the tube is 0.5cm and the fluid is "viscous" water (ρ=1.0, σ=70, μ=0.1) with a contact angle of 30°. Here again viscosity is increase by a factor of ten to damp capillary waves. Gravity is negative 980.0cm/s^2 in the z-direction.

A simulation, Fig.3,was made using a uniform grid of elements of edge length 0.025cm and using symmetry in x and y directions so that only the first quadrant of the flow needs to be simulated. The theoretical amount of fluid pulled up the tube in one quadrant is again determined by the balance between wall adhesion and gravity,

$$Vol = \frac{\sigma \cos(30) w}{\rho g},$$

Where *w* in this case if the length of the side wall 0.707cm resulting in a prediction of the amount of water volume raised by capillary action to be Vol=0.04373.

The simulation result was a lifted water volume of 0.04373cc, or the exact theoretical amount when using an *fclean*=0.2. Repeating these simulations with the alternative secular instability treatment (***ifloss=1***) gives a volume of 0.09% low. Doubling the resolution and using *fclean*=0.0 resulted in a volume of 0.46% below theory. Including the ***ifloss=***1 option resulted in a volume of 0.12% below theory. For the original simulation a value of *fclean*=0.2 was used, but this was reduced to zero for the better resolved case. It was also found that better results are obtained using the VOF advection option of *ifvof=3*, instead of the default value *ifvof=4*.

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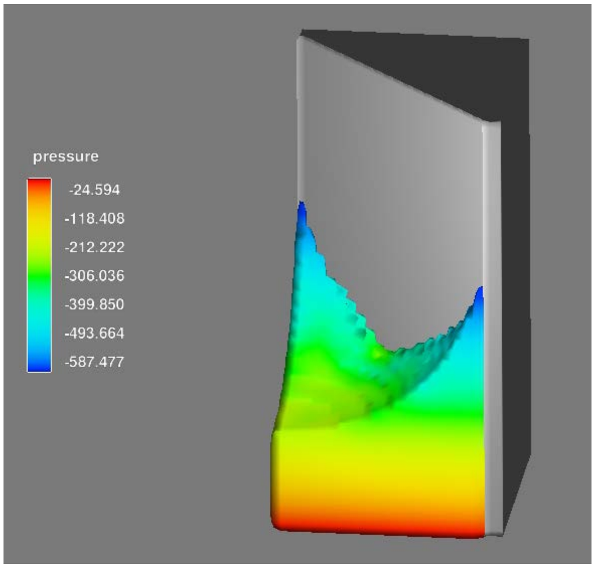

Figure 3. Capillary rise in square tube rotated 45° in rectangular grid.

Case 4: Capillary rise in a circular tube embedded in a rectangular grid.

The fourth test case is another capillary rise problem, but for a simple cylindrical tube of radius 0.05cm containing a made up fluid of density 1.0gm/cc, having a surface tension coefficient of 100dynes/cm and a viscosity of 0.025gm/cm/s. The contact angle with the side wall of the tube is 30° and gravity is down with a value of 1000cm/s^2. Both the top and bottom of the computational grid are fixed pressure boundaries with zero pressure.

What makes this test somewhat different from the previous test is that it is a circular tube placed in a grid of rectangular elements, so that the wall of the tube is intersecting the grid cells all along its circumference, creating a series of partially blocked grid elements where the blockage varies from little to nearly an entire element.

The theoretical amount of fluid that should be raised up in the tube is

$$Vol = \frac{\sigma \cos(30) w}{\rho g},$$

where w in this case is $0.05\pi/2$ giving Vol=0.0068cc.

An initial simulation was made using a uniform grid of elements of edge length 0.01cm (i.e., 5 cells across the inner radius of the tube). Because of symmetry only a 90° quadrant was modeled. The amount of fluid raised was 0.0613 or 9.8% below the theoretical value. When the simulation was repeated with 8cells across the tube radius the amount of fluid raised was 0.0604 or 11.1% below the value predicted analytically. Figure 4 shows the top portion of the fluid in the tube at the end of the simulation when the fluid rise has reached its equilibrium height.

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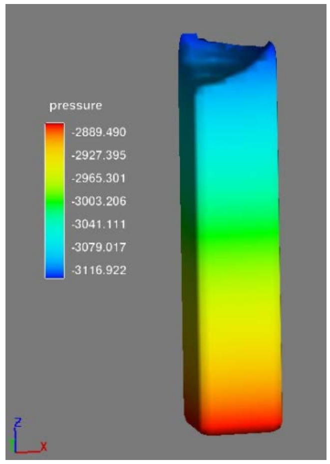

Figure 4. Top portion of fluid raised in a cylindrical tube by capillary action.

The differences between these results and the analytic solution, when compared with the previous test cases, are larger than expected. Considerable effort has been expended to determine why adhesion on obstacle surfaces within mesh elements, as opposed to surfaces on the faces of elements, should result in less capillary rise. Every detail of the model appears to be working correctly (e.g., the correct amount of adhesion force is being computed in every element). The computed interface appears to be smooth and reasonable, and there are no extraneous bits of fluid being shed from the surface.

The simulation results are not so far off as to discredit the overall surface tension model, which is working very well for a wide range of applications. However, more work is being done to pin point why this particular problem in not working as well as expected.

Case 5: Capillary rise in a cylindrical tube in a cylindrical grid.

The test surface tension modeling in cylindrical coordinate grids the previous test case has been repeated with a 90° section of a cylindrical grid, Fig.5. The outer radius is 0.05cm and there are no partially blocked grid elements. However, because the grid elements converge at the origin creating small cell sizes that cause the time-step size to be quite small (order 5.0e-7s), which leads to a long CPU time (order of several days). The volume of fluid raised is 0.00692cc, which is 1.8% above the theoretical prediction of 0.0068cc. A view of the top most portion of the fluid is shown in the right frame of Fig.5.

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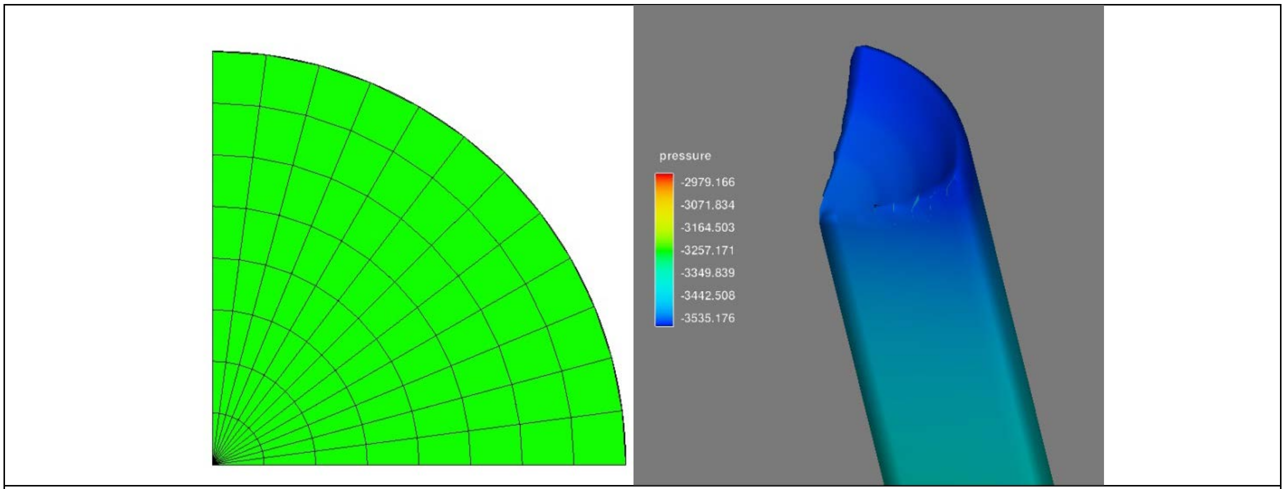

Figure 5. Cylindrical grid used to model a 90° cross section of a cylinder (left) and top portion of cylindrical fluid raised by capillary action.

Case 6: Capillary Rise in an annular tube in a cylindrical grid.

The previous test case has been repeated with the replacement of the central region with a solid cylinder having a radius of 0.01875cm. A solid outer cylinder has also been added with an inner radius of 0.05cm, as shown in Fig.6. The axial grid is uniform with elements of height 0.00625cm.

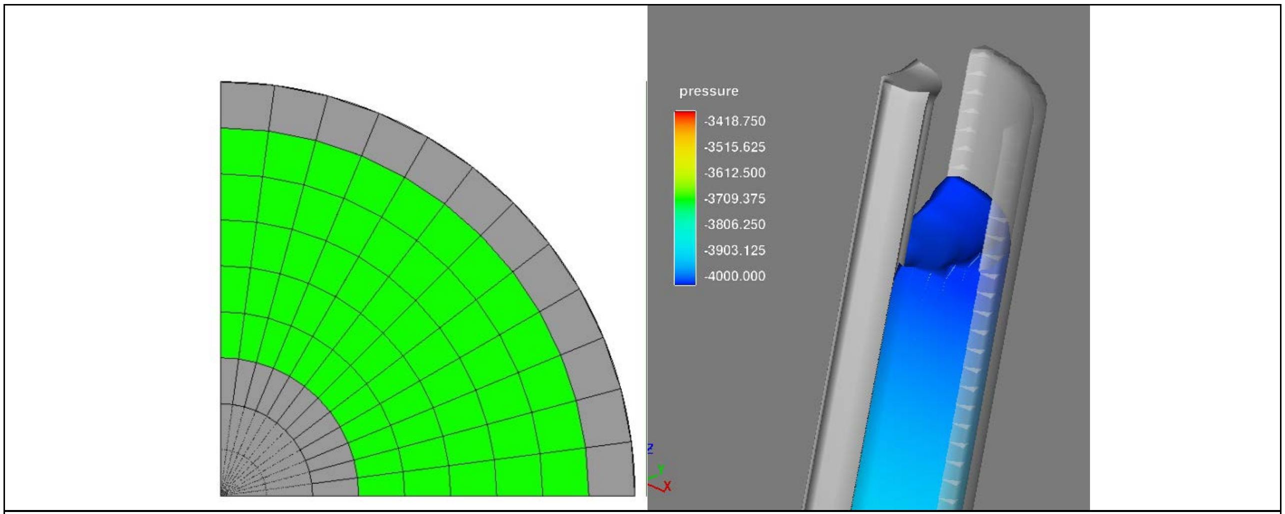

Figure 6. Cylindrical grid used to model a 90° cross section of a cylindrical annulus (left) and top portion of equilibrium fluid column (right).

The advantage of the cylindrical grid is that the walls of the annular tube coincide with grid lines, so here again there are no partially blocked elements.

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All parameters are as in the previous example with 5 elements across the annulus. However, the contact angle on the inner wall is 90° while that on the outer wall remains at 30°.

This simulation resulted in a capillary rise of volume of 0.00674cc, which is 0.9% below the theoretical value of 0.0068cc. The top surface of the fluid has a nice smooth configuration with no extraneous bits of fluid floating about.

Appendix: Comments about a new treatment for secular instabilities.

It was mentioned in **Case 2** that there is a new technique for the elimination of secular instabilities. Briefly, a secular instability is a situation where one or more velocity components exhibit a monotonic growth of magnitude in time. This is typically caused by the existence of an acceleration term (e.g., gravity or a fixed pressure gradient) that is not opposed by any resistance (e.g., viscosity or fluid advection). To compensate for such situations, although rare, a technique was introduced in the early life of ***FLOW-3D*** that modified some velocities existing in locations where secular behavior was considered possible. A disadvantage of this scheme was that it could occasionally introduce some localized unphysical behavior, even when secular instabilities were not developing.

A new technique referred to as FAVOR™ Losses, has been introduced to replace and refine the treatment of secular behavior. In this technique, the program is monitored through the Mentor routine to identify possible secular behavior. If such behavior is identified then a small flow loss is introduced at the problem location. In most cases this is sufficient to eliminate the secular behavior, but if not, then the flow loss magnitude is made a little larger and can be further increased if necessary for up to four times. Such losses are also removed should the possibility of a secular instability at a particular location is no longer possible. The advantage of this new technique is that the flow is only modified at specific locations and only if a secular behavior is occurring at that location. Furthermore, the loss additions are kept as small as possible and even removed when no longer needed. Thus, the corrective modifications to the flow advection logic are kept to a minimum.

To use this new feature the user must request it by introducing the parameter ***ifloss***=***1*** in the input file. Eventually, this will be made a default setting when no reports of problems are reported from its use.

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