Using Surface Evolver to Model the Behavior of Liquid Deuterium

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Abstract

Successful exploitation of laser fusion as an energy source requires that laser targets be produced quickly on an assembly-line basis. The final step in fabricating a laser target is the fueling operation, where cryogenic liquid deuterium is loaded into thin polymer shells. This fueling must be done remotely because liquid deuterium must be maintained at around 20 Kelvin. It is required that precise volumes of liquid deuterium are dispensed, on the order of 90 microliters per target. This task is complicated because liquid deuterium has a contact angle of zero (perfectly wetting), behaving differently from other, more familiar liquids, such as water. To address this issue, this work used “Surface Evolver,” a software tool developed by K. Brakke that uses energy minimization to evolve fluid shapes into their final equilibrium forms subject to surface tension, gravity, and other forces. The behavior of liquid deuterium between parallel plates was modeled, including parallel vertical plates with varying widths and non-parallel horizontal plates. The parallel plate geometry is favored because electrodes can be attached to the plates for precise manipulation and dispensing.

Introduction

At the Laboratory for Laser Energetics, the OMEGA-60 laser is used primarily to conduct fusion reactions. These fusion reactions involve using 60 laser beams to hit a small, cryogenic target inside the target chamber. These targets need to be fueled with cryogenic liquid deuterium into thin polymer shells. The current batch process for making these laser targets is rather slow, but it is still fast enough for the experiments. However, if laser fusion were to be used as an energy source, the targets would need to be produced on-site much quicker because the laser would need to be fired many times per minute.

Cryogenic liquid deuterium has a special property in that it has a zero contact angle, meaning that it is perfectly wetting. In order to better understand the behavior of cryogenic liquid deuterium, we can use a program called “Surface Evolver” to simulate its behavior. After giving it an initial input file that defines the initial shape of a body, the program will then output an evolved profile, which should be the one of minimum energy.

The simplest example is the evolution of a cube into a sphere, as shown in Fig. 1. “Surface Evolver” starts with an input file of a cube, which is representative of a cube of liquid in free space. In this simple example, the governing equation is $E = \gamma A$, where E is the energy that we want to minimize, γ is the surface tension (which is constant), and A is the contact area. To minimize the energy, we want to minimize the contact area since the surface tension is constant. A sphere of volume 1 m^3 has a total surface area of 4.83 m^2, whereas a cube with the same volume has a total surface area of 6 m^2. Because the three-dimensional shape that has the smallest surface area is a sphere and not a cube, Surface Evolver will gradually evolve the cube into a sphere. This is why droplets in midair are more spherical and never cubes. In seeking the minimum energy state, “Surface Evolver” uses a series of commands including “refine,” which increases the total number of vertices, and "go," which processes the current body and tries to minimize the total energy using a gradient descent method. As the shape is further refined, the body approaches the shape of a perfect sphere.

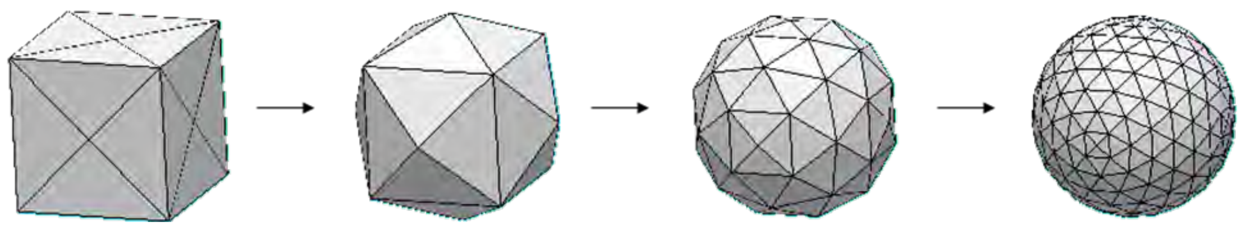

Figure 1: Process used by Surface Evolver to model the simple evolution of a cube into a sphere.

Similar to the above example, "Surface Evolver" can also model the behavior of liquid deuterium between two parallel plates. Given an initial shape, the program will evolve it and output a profile for the cryogenic liquid deuterium in between those two parallel plates, as shown in Fig. 2.

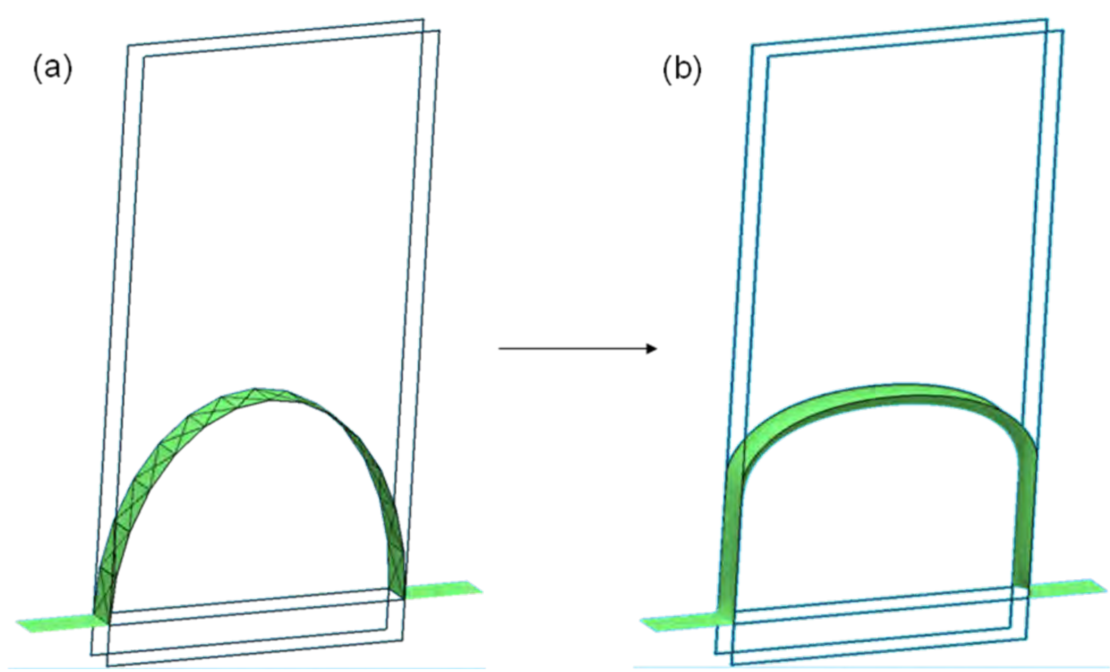

Figure 2: (a) Initial meniscus profile given to Surface Evolver and (b) meniscus calculated by Surface Evolver.

Effect of Plate Width on Meniscus Height-of-Rise

The maximum height-of-rise of the meniscus, which occurs at the center of the plates, varies with the plate width. Some convenient measures of the height of the meniscus at the displacement from the center *x* are labeled in Fig. 3.

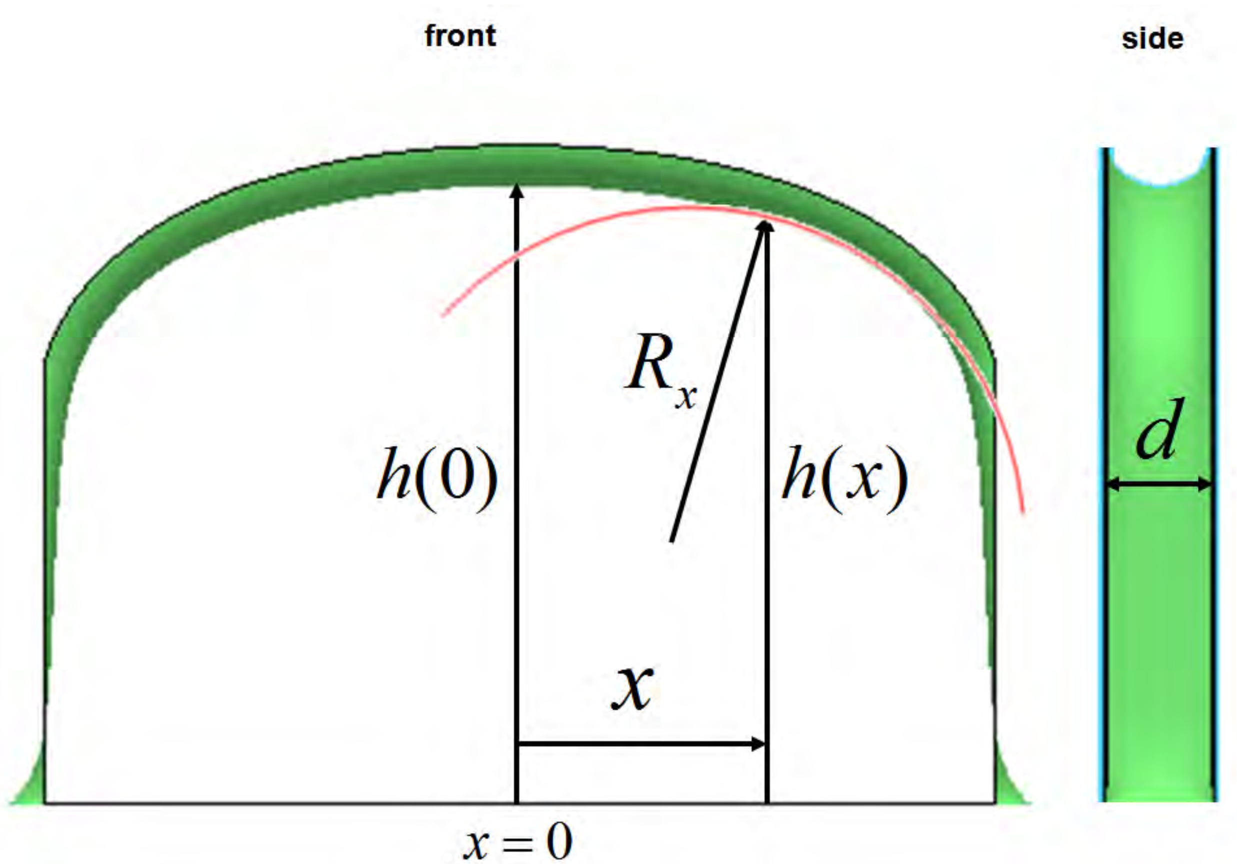

Figure 3: Properties of the meniscus used in Eqn. 1.

The following equation governs the height-of-rise as a function of *x*, the displacement from the center of the plates:

$$h(x) = \frac{\gamma \cos(\theta_c)}{\rho g}\left(\frac{2}{d} - \frac{1}{R_x}\right) \quad (1)$$

In Eqn. 1, $h(x)$ is the height of the meniscus, γ is the surface tension, θ_c is the contact angle, ρ is the density of the fluid, g is the acceleration due to gravity, d is distance separating the two parallel plates, and R_x is the radius of curvature at the position on the plate. In this experiment, the primary interest is in $h(0)$, the height-of-rise at the center of the plate.

For this "Surface Evolver" simulation experiment on the effect of the plate width on the maximum meniscus height-of-rise, the temperature was held at a constant 18.7 Kelvin. It is important to note that both the surface tension and the density of the liquid are dependent on the temperature. At this temperature, the surface tension is 0.00382 J/m^2 and the density is 174 kg/m^3. Other constants included the gravitational acceleration, which was 9.81 m/s^2, and the plate separation, which was 0.86 mm. As the plates became wider, the radius of curvature at the center increased towards infinity. From Eqn. 1, that made the height-of-rise increase towards its maximum, which occurs when the meniscus is perfectly flat and the radius of curvature is infinity.

"Surface Evolver" does indeed give those results, as shown in Fig. 4. The wider plates have a higher height-of-rise at the center of the plates. The wider plates also have a much flatter region in the center where the radius of curvature approaches infinity.

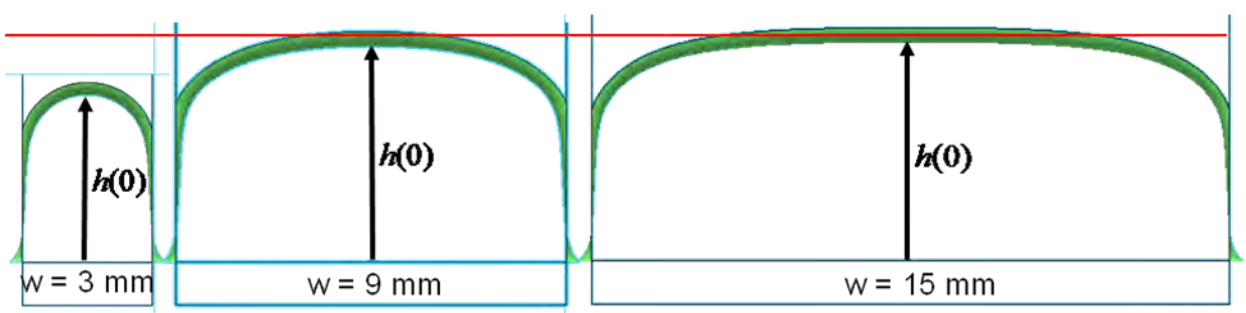

Figure 4: Calculated meniscuses for three different plate widths. The deuterium rises higher between wider plates, but levels off as the plates become wider. The red line marks the theoretical maximum height of rise.

Comparison of measured profiles to theory

After “Surface Evolver” generated a meniscus profile, data was extracted to see whether the radius of curvature was consistent with the height as predicted by Eqn. 1. There were two ways to extract the data: using a dump-file from “Surface Evolver” containing all the three-dimensional coordinates and saving a bitmap from a screenshot of the profile. It was necessary to find the second derivative of the meniscus profile to calculate the radius of curvature. The following equation describes how to calculate the radius of curvature:

$$R_x = \frac{\left[1+\left(\frac{dy}{dx}\right)^2\right]^{3/2}}{\left|\frac{d^2y}{dx^2}\right|} \tag{2}$$

In Eqn. 2, R_x is the radius of curvature, dy/dx is the first derivative, and d^2y/dx^2 is the second derivative of the function $y(x)$.

Because “Surface Evolver” uses a numerical method instead of an analytical method to solve for the configuration of lowest energy, the values for the points are not exact. Furthermore, the bitmap had additional numerical noise because the measurements were limited by the pixel resolution.

Since the bitmap method has pixels evenly spaced out along the *x*-axis, a first derivative could be numerically obtained at some point by taking the slope between the two points immediately to its left and right. The second derivative could be calculated using this same method on the points from the first derivative. However, this yielded extremely noisy and thus meaningless results. The unsmoothed second derivative had most of its values between ±50,000 compared to the smoothed second derivative, which only ranged between –100 and –350.

To address this matter, a MATLAB program was written to smooth out the curve. This smoothing algorithm can reduce the numerical noise enough so that the results from the data extracted from both the dump-file and the bitmap image are sufficiently smooth. The smoothing algorithm takes the first n points starting with the first point on the curve and fits a line to it. Thus, a value for the first derivative, or the slope of the best-fit line, can be obtained at the average of the x-values for the first n points. We can repeat this process for the next n points starting at the second point, then the third point, and so on.

To get the smoothed second derivative, this same algorithm was applied on the points obtained for the first derivative. Due to the nature of this smoothing algorithm, it takes off points on both the left and right ends of the curve it is smoothing. This loss of side points does not significantly affect our analysis because the primary focus is on the meniscus at the center of the plates. There are remarkable differences between the unsmoothed first and second derivatives, as shown in Fig. 5. Whereas the unsmoothed second derivative is so noisy that no real meaning can be gotten from it, the smoothed second derivative is very well-behaved.

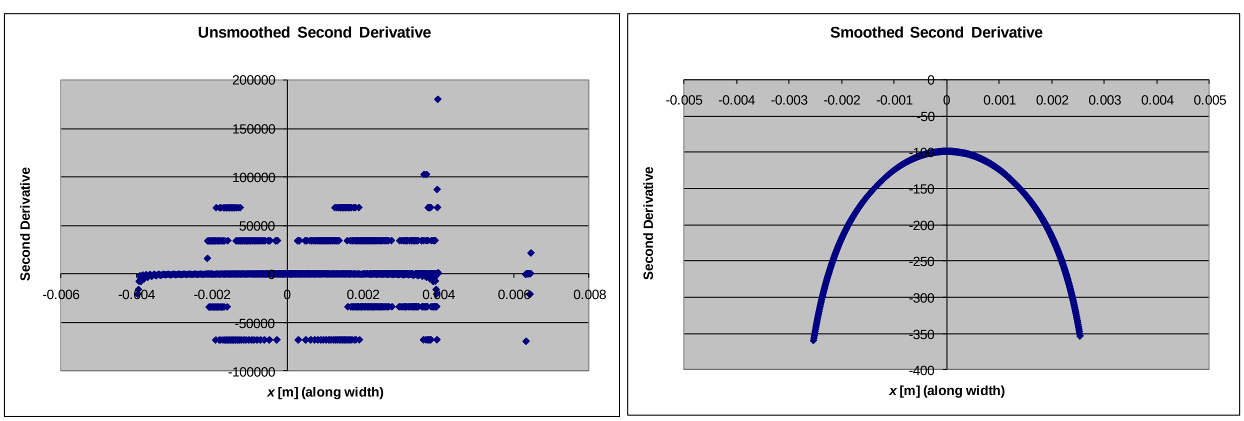

Figure 5: Comparison of the unsmoothed and smoothed second derivative. The unsmoothed curve has a huge range of values, and such a large distribution of the points makes it meaningless. On the other hand, the smoothed curve had a much smaller range and looks reasonable. Note that the smoothed curve does not extend as far as the unsmoothed one. The right-most point on the smoothed curve is at around 0.0025 m, whereas the right-most point on the unsmoothed curve reaches around 0.0040 m.

To get the points from "Surface Evolver," the image method was preferred over the dump-file method because the picture had evenly spaced pixels whereas the dump-file contained points scattered at irregular intervals due to "Surface Evolver" using a numerical method. Having the points at set intervals apart made it much easier to numerically calculate the curvature, which is required for the predicted meniscus height-of-rise. Also, after many refinements, the dump-file would have many more points than were actually needed. Even though the precision of the bitmap method was limited to the resolution of the image, the smoothing algorithm made the smoothed-out bitmap calculation virtually the same as the smoothed-out dump-file calculation, as shown in Fig. 6.

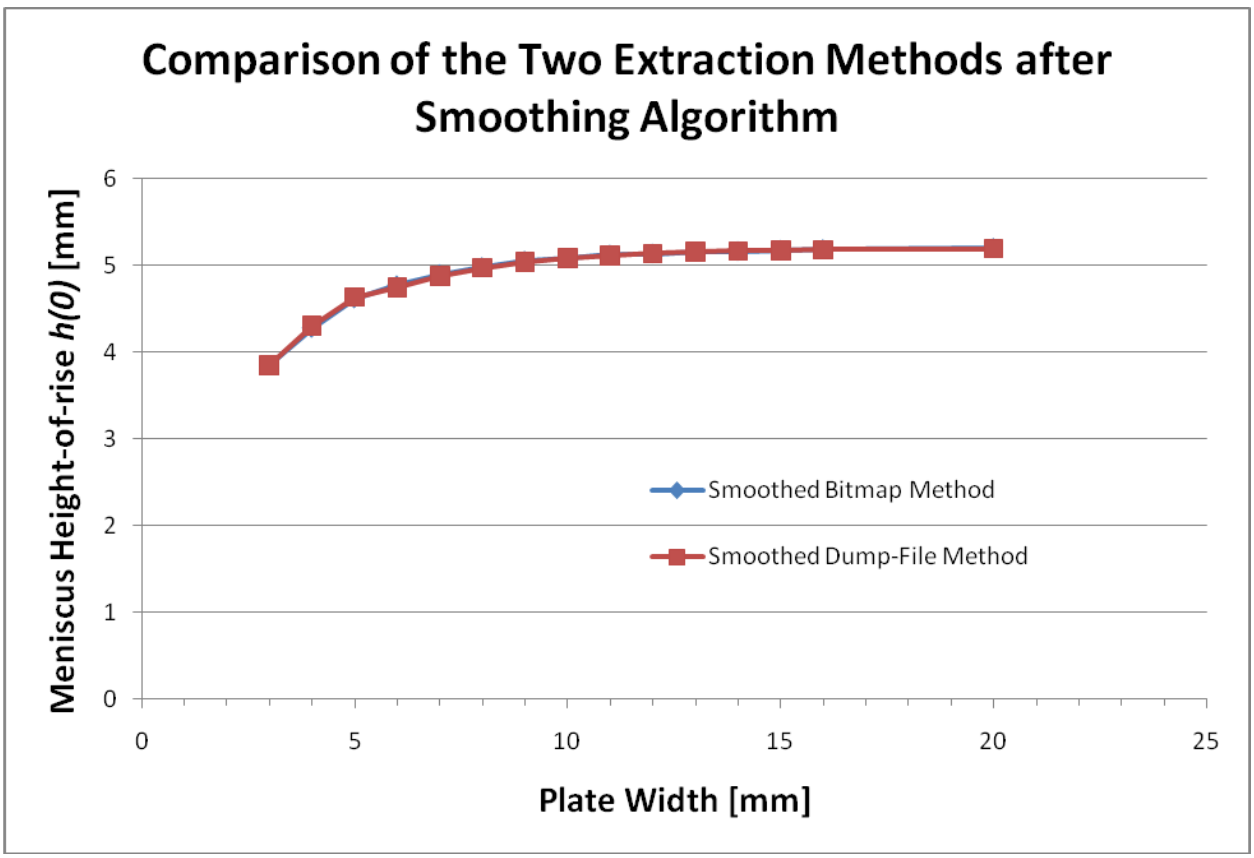

Figure 6: Calculated meniscus height as a function of plate width. The blue points, which are largely obscured because the blue line is virtually the same as the red line, are calculated heights from the smoothed bitmap using Eqn. 1. The red points have been obtained from calculating the same height-of-rise from the smoothed dump-file using Eqn. 1. Because the two line up so well, the two methods yield basically the same results, which is expected since the data itself is inherently the same, just extracted using different methods.

Results

After applying the smoothing algorithm, the radius of curvature could be calculated by substituting the first and second derivatives into Eqn. 2. This enabled a predicted meniscus height to be calculated using Eqn. 1. Both this curve calculated using Eqn. 1 and the curve directly extracted from "Surface Evolver" are very similar, as shown in Fig. 7. For wider plates, the calculated and extracted curves line up almost exactly, but for smaller plates such as 3 millimeters, the calculated curves are slightly under the extracted ones, most likely due to the smoothing algorithm not being able to handle fewer points or "Surface Evolver" having trouble calculating the profile under the edge effect near the edges of the plates. For very wide plates, for example, 16 millimeters, the calculated results are slightly above the extracted results. Overall, the calculated and extracted curves are very close for all cases.

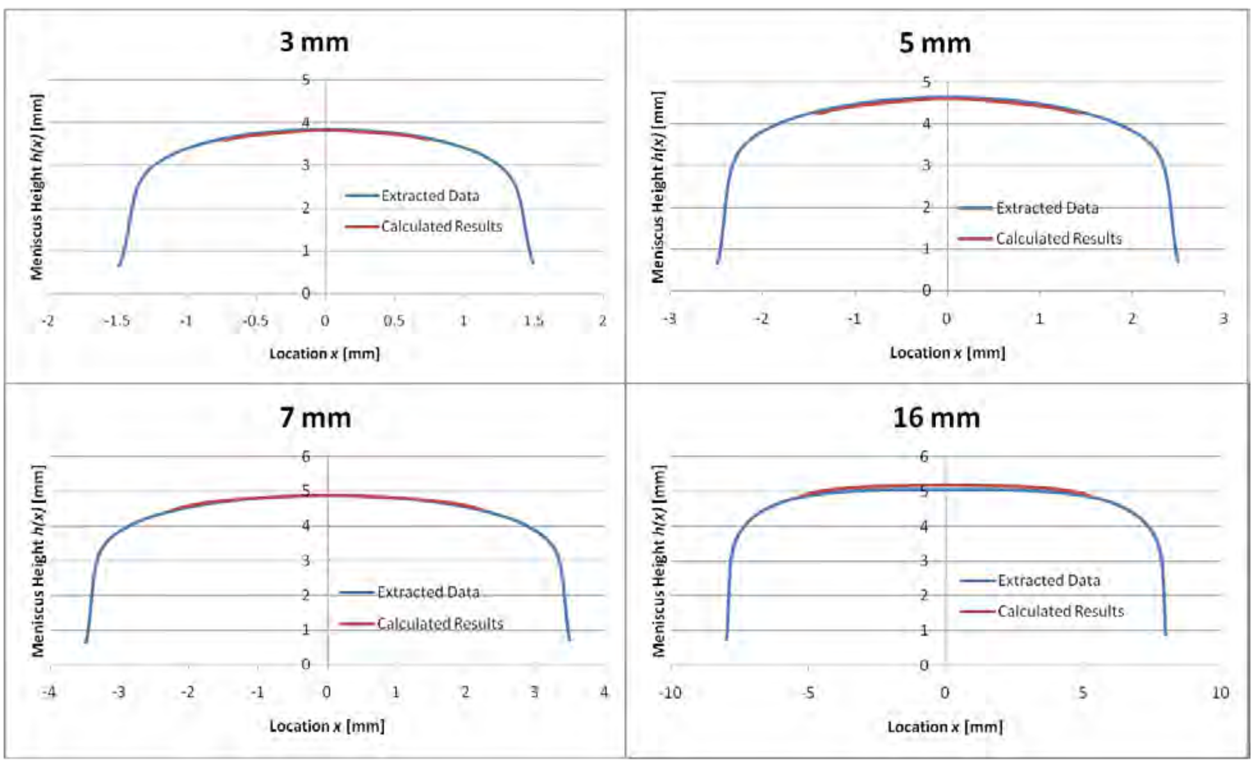

Figure 7: The comparison of the extracted data and calculated results for several different plate widths. As shown, they all line up very well, showing that "Surface Evolver" is consistent with the calculations based on Eqn. 1. The smaller plates have the extracted data slightly under the calculated result, whereas the larger plates have a slightly higher calculated result compared to the extracted data.

A comparison of the height of the meniscus at the center position (x = 0 in Fig. 7) obtained by the two methods is given in Fig. 8, where the maximum height-of-rise is plotted against the plate width. The two line up very closely, indicating that "Surface Evolver" is indeed calculating the profile correctly, as shown in Fig. 8. It is possible to see the trend that the meniscus maximum height-of-rise for narrower plates is not as high as that of the wider plates. Also, it is noticeable that the meniscus height eventually levels out such that all of the maximum heights after around a plate width of 10 millimeters are approximately the same. Performing a logistic regression on the data, a best-fit curve was obtained for the meniscus height-of-rise at the center as a function of plate width for the given temperature and plate separation distance, where h_{max} is the height of the meniscus in meters and w is the width of the plate in meters:

$$h_{\max} = \frac{0.005045}{1 + 1.767e^{-576.7w}} \tag{3}$$

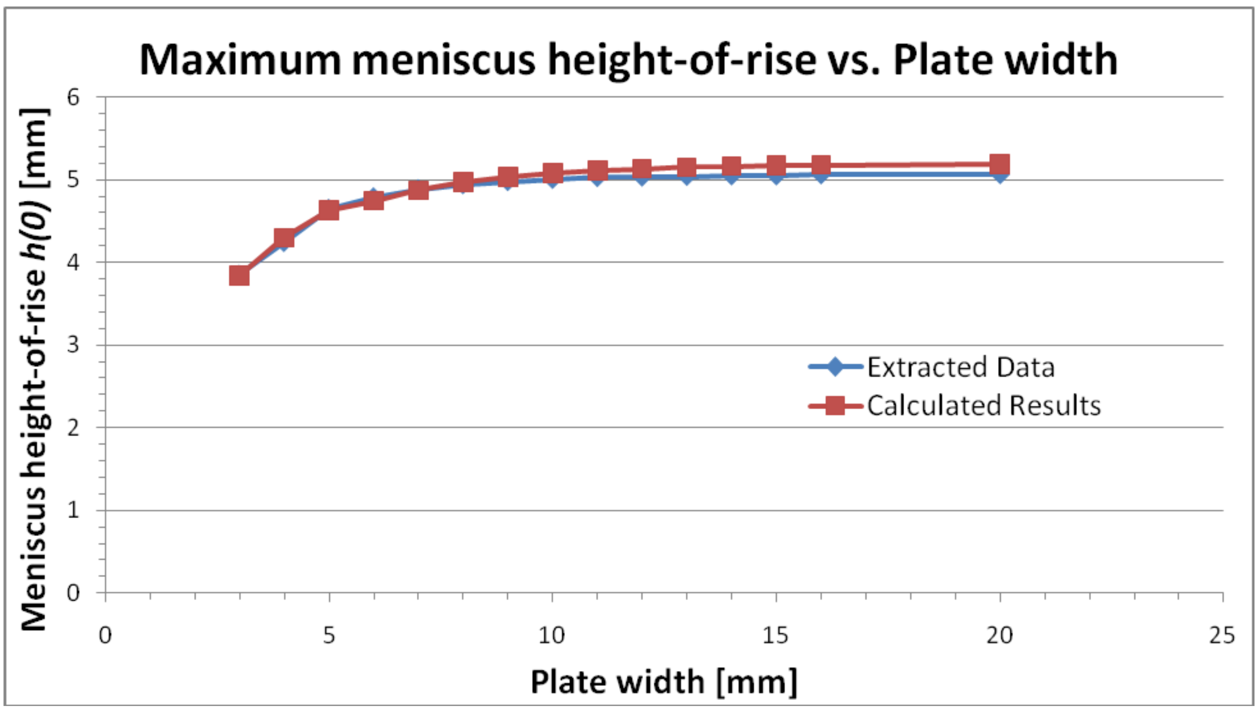

Figure 8: Meniscus height as a function of plate width. The blue points are heights measured directly from "Surface Evolver" results such as the ones in Fig. 4. The red points have been obtained by measuring the curvature of the "Surface Evolver" profile and substituting it into Eqn. 1. The close agreement shows that the "Surface Evolver" results are consistent with Eqn. 1.

Surface Evolver helps understand how cryogenic liquid deuterium behaves between two parallel plates. The parallel plate geometry is desirable because it is much easier to attach electrodes onto flat plates than to put them on other shapes, such as a cylindrical tube. An applied voltage will then be able to draw up the liquid further, which is called liquid dielectrophoresis.[1] Being able to use a voltage to control the movement of the liquid deuterium is a viable method of moving it remotely at cryogenic temperatures.

This voltage can increase or decrease the amounts of liquid deuterium by very small amounts. It is hoped that this can be used to manipulate the liquid deuterium and dispense very small amounts of it with good accuracy.

Movement of a Droplet between Horizontal Plates

A droplet of liquid between two perfectly horizontal plates will stay put between the plates, but if the plates are not parallel to each other, then the droplet will tend to move. For hydrophobic droplets, which have contact angles greater than 90°, the droplet will begin to move towards the diverging area of the plates. For hydrophilic droplets, which have contact angles less than 90°, the droplet will begin to move towards the converging area of the plates, as shown in Fig. 9.

This setup is not as amenable to “Surface Evolver” because this seeks to actually move the droplet around whereas the previous experiment obtained an equilibrium position of the same deuterium between the plates. However, “Surface Evolver” will still move the droplets in the correct directions based on their contact angles. Although the droplet is moving in the correct direction, it is not doing so as a function of time because the evolutions are on a gradient descent method, not as an evolution with time.

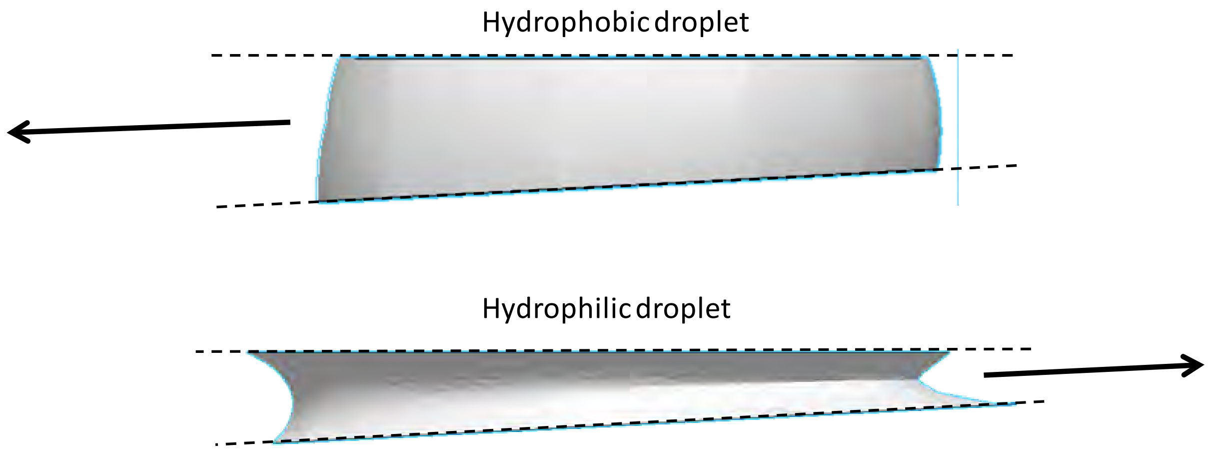

Figure 9: The movement of a hydrophobic droplet and a hydrophilic droplet. The hydrophobic droplet is in a wider region of the plates and is moving towards the diverging area. The hydrophilic droplet is in a narrower region of the plates and is moving towards the converging area. Note that the textures on the two droplets do not look smooth because "Surface Evolver" is not good at physically moving droplets; instead it just seeks out an equilibrium shape.

Liquid deuterium is an extremely hydrophilic droplet because it has a contact angle of 0°, so it will move towards the narrower area between the plates. Because of this behavior, it is possible to transport miniscule volumes of cryogenic liquid deuterium to meet the target shells using horizontal plates after a specific volume has been measured out and dispensed.

Also, a voltage can be applied by attaching electrodes onto the plates. As before, the voltage will change the behavior of the liquid deuterium, allowing greater control over its movement so that it can be ultimately dispensed and transported manually into target shells.

Due to the effect of electrowetting, the applied voltage will increase the contact angle of a hydrophilic droplet such as liquid deuterium,[2] so that it can still be moved around once it exits the horizontal parallel plates.

Conclusion

"Surface Evolver" is very effective in modeling the behavior of cryogenic liquid deuterium in a vertical parallel plate geometry. MATLAB was used to process the data from "Surface Evolver," which produced accurate results that are consistent with the theoretical predictions regarding the meniscus height-of-rise. By using this software tool, it is possible to see the effects of the plate width on the maximum meniscus height-of-rise, which occurs in the middle of the plate. Although "Surface Evolver" is not well-suited for showing the behavior of a droplet of liquid between two horizontal, non-parallel plates, the computer program is able to show both the general shape of the droplet and the direction it will move based on the plate misalignment angle and the contact angle between the plates and the droplet. Gaining a better understanding of the behavior of liquid deuterium can aid in the design of an effective assembly-line method to build and transport laser targets on-site to make laser fusion become a viable energy source in the future.

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References

[1] T. B. Jones, R. Gram, K. Kentch, D. R. Harding, "Capillarity and dielectrophoresis of liquid deuterium," *J. Appl. Phys.* **42**, 225505 (2009).

[2] C. Roero, "Contact angle measurements of sessile drops deformed by a DC electric field," Proc. of 4th International Symposium on Contact Angle, Wettability and Adhesion, Philadelphia, USA, 2004.