

Owens-Wendt Surface Energy Calculation

The Owens-Wendt geometric mean equation

$$(1 + \cos(\theta)) \gamma_{LV} = 2 \sqrt{(\gamma_S^D \gamma_L^D)} + 2 \sqrt{(\gamma_S^P \gamma_L^P)}$$

is one method, of many, of estimating surface free energy from contact angles. It is important to understand that there is not necessarily an exact solution to the equation. Why is this so? Because the contact angle data you supply may not be self-consistent. Recall that contact angles are always associated with their adjacent test liquids, and the chemistry of these liquids demands a certain response from the sample. If, through experimental error, one or more of the angles is not correct, then a normal solution may not exist.

A second, and related, aspect is whether repulsive forces are present. These would carry negative values in the equation (adhesive forces are positive). Negative values require special consideration when you take the square root. FTA software allows you to choose whether to allow negative values and it then solves the equation numerically using a regression approach. This means you get the *best available answer given the circumstances*. We report the residual, which is the statistical error in the solution, so you can judge the quality of the answer. The residual is in surface energy units, so a residual of 1 is approximately 1/18 the energy of Teflon and 1/72 the tension of water. Larger residuals, such as those over 1, are flagged as suspect. Even though there may be no good solution, the reported solution is the best you can get under the circumstances.

As an example, let us consider some data reported to us, probably data from a super-hydrophobic surface.

Water angle: 135.743°

Methylene iodide angle: 106.602°

The Fra32 Surface Energy Calculator screen is shown on the next page. The handbook values for water and methylene iodide are shown in the topmost table, on lines 1 and 4 respectively. The contact angle data for the case at hand has been entered on lines 3 and 4 of the middle table. The proposed surface energy solution appears on line 3 of the bottom table. It is highlighted. Notice that there is a checkbox in the lower right “Allow energies < 0”. It is checked in this screen shot. This means to allow negative values of energy in the solution. The calculation status bar says that there are “One or more negative values” and the residual is some very small number.

The screenshot shows the Fta32 Video 2.0 software interface. The main window is titled "Surface Energy" and contains three data tables. The first table, "Liquid Data", lists properties for Water, Air, Formamide, and Methylene Iodide. The second table, "Contact Angles", shows contact angles for Methylene Iodide and Water on Plastic1 and Jasco samples. The third table, "Surface Energies and Adhesions", shows results for the Owens and Zisman methods on Plastic1 and Jasco samples. The "Dynamic IFT" section shows a calculation for the wetting tension of liquid to solid, resulting in a residual of 0.000002.

Index	Liquid	Formula	Density	IFTension	Dispersive	Polar	Acid	Base
1	Water	H2O	0.9982	72.80	21.80	51.00	25.50	25.50
2	Air		0.0011	0	0	0	0	0
3	Formamide	H3CON	1.1300	58.00	39.00	19.00	2.280	39.60
4	Methylene Iodide (MI)	CH2I2	3.3200	50.80	50.80	0	0	0

Index	Test Liquid	Sample	Angle	IFTension	Dispersive	Polar	Acid	Base
2	Methylene Iodide (MI)	Plastic1	57.20	50.80	50.80	0	0	0
3	Water	Jasco	135.74	72.80	21.80	51.00	25.50	25.50
4	Methylene Iodide (MI)	Jasco	106.60	50.80	50.80	0	0	0

Index	Method	Sample	ContactAngles (by Index)	IFT (Energy)	Dispersive	Polar	Acid	Base
1	6.Owens	Plastic1	1, 2	32.07	30.19	1.881	0	0
2	2.Zisman	Plastic1	1, 2	33.05	0	0	0	0
3	6.Owens Geo	Jasco	3, 4	6.432	6.479	-4.743E-2	0	0

6.Owens Geo One or more negative values, residual = 0.000002

1. Wetting Tension of liquid to solid (cosine of angle multiplying liquid IFT): 1 angle of 1 fluid on 1 solid

The dispersive result (γ_S^D) is 6.432mN/m and the polar result (γ_S^P) is -0.0474mN/m.

Notice the handbook values for the test liquids. If you use different values, your results will be different.

We also ran this under the assumption that negative energies were not allowed. The results are shown on the next page. The dispersive result is 6.047mN/m and the polar result is 0. But the residual is now 1.847mN/m, a considerable fraction of the answer. Which do you prefer: high residual or negative values? Not a nice choice.

Another worker proposed that the correct answer was 7.25 dispersive and 0.09 polar. Let's substitute all three sets (FTA with negative values, FTA without negative values, and customer's) back into the original equation set and see how they balance.

The screenshot shows the Fta32 Video 2.0 software interface. The main window is titled "Surface Energy" and contains three data tables. The first table, "Liquid Data", lists properties for Water, Air, Formamide, and Methylene Iodide (MI). The second table, "Contact Angles", lists contact angles for Methylene Iodide (MI) on Plastic1 and Water on Jasco. The third table, "Surface Energies and Adhesions", lists dynamic IFT values for Owens and Zisman methods on Plastic1 and Jasco. Below the tables are control buttons for "Set Liquid", "Add Row", "Sort by Index", "Sort by Col", "Delete Row", and "Clear Table". At the bottom, there is a text input field with the value "6.Owens Geo No good solution, residual = 1.847114" and a "Calc" button.

Index	Liquid	Formula	Density	IFTension	Dispersive	Polar	Acid	Base
1	Water	H2O	0.9982	72.80	21.80	51.00	25.50	25.50
2	Air		0.0011	0	0	0	0	0
3	Formamide	H3CON	1.1300	58.00	39.00	19.00	2.280	39.60
4	Methylene Iodide (MI)	CH2I2	3.3200	50.80	50.80	0	0	0

Index	Test Liquid	Sample	Angle	IFTension	Dispersive	Polar	Acid	Base
2	Methylene Iodide (MI)	Plastic1	57.20	50.80	50.80	0	0	0
3	Water	Jasco	135.74	72.80	21.80	51.00	25.50	25.50
4	Methylene Iodide (MI)	Jasco	106.60	50.80	50.80	0	0	0

Index	Method	Sample	ContactAngles (by Index)	IFT (Energy)	Dispersive	Polar	Acid	Base
1	6.Owens	Plastic1	1, 2	32.07	30.19	1.881	0	0
2	2.Zisman	Plastic1	1, 2	33.05	0	0	0	0
3	6.Owens Geo	Jasco	3, 4	6.047	6.047	0	0	0

Original equation, written for both water and methylene iodide, below. The left hand side will be the same for all three candidates since the contact angles are the same.

$$(1 + \cos(\theta)) \gamma_{LV} = 2 \sqrt{(\gamma_S^D \gamma_L^D)} + 2 \sqrt{(\gamma_S^P \gamma_L^P)}$$

FTA, Negative Values:

Substituting in, we have for water first and methylene iodide second,

$$(.283783) 72.8 = 2 \sqrt{(6.432 \times 21.8)} + 2 \sqrt{(-0.0474 \times 51)}$$

$$(.712278) 50.8 = 2 \sqrt{(6.432 \times 50.8)} + 2 \sqrt{(-0.0474 \times 0)}$$

$$20.659 = 23.682 - 3.109 = 20.572 \text{ (applying negative values repulse)}$$

$$36.285 = 36.152 + 0 = 36.152$$

Unbalances in equations are 0.087 and 0.133.

FTA, No Negative Values:

$$(.283783) 72.8 = 2 \sqrt{(6.047 \times 21.8)} + 2 \sqrt{(0 \times 51)}$$

$$(.712278) 50.8 = 2 \sqrt{(6.047 \times 50.8)} + 2 \sqrt{(0 \times 0)}$$

$$20.659 = 22.963 + 0 = 22.963$$

$$36.285 = 35.053 + 0 = 35.053$$

Unbalances in equations are -2.304 and 1.232.

Customer's

$$(.283783) 72.8 = 2 \sqrt{(7.25 \times 21.8)} + 2 \sqrt{(0.09 \times 51)}$$

$$(.712278) 50.8 = 2 \sqrt{(7.25 \times 50.8)} + 2 \sqrt{(0.09 \times 0)}$$

$$20.659 = 25.144 + 4.284 = 29.428$$

$$36.285 = 38.382 + 0 = 38.383$$

Unbalances in equations are -8.769 and -2.097. As it stands, this is the worst fit.