

Supplementary material

Analysis of Distillate Fractions Collected from a Small Commercial Pot Still Using NMR and GC-MS

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Table S1. Fractions from 5 gallon Vevor pot still.

Fraction	Collected volume (mL)	T ^a (°F) run #1	Proof run #1	T ^a (°F) run #2	Proof run #2	T ^a (°F) run #3	Proof run #3	Notes
#1	100	180	162	182	162	180	156	
#2	200	180	159	186	157	181	156	
#3	200	181	154	189	147	181	150	
#4	200	180	145	190	131	182	143	
#5	200	184	134	190	114	182	135	
#6	200	187	123	190	101	183	126	
#7	200	187	113	190	92	184	118	
#8	200	189	104	190	86	185	110	
#9	200	190	93	190	79	187	102	Run #2-cloudy, blue matter
#10	200	190	85	192	70	189	95	Run #1, #2-cloudy; Run #2-blue matter

^aTemperature read directly from thermometer on top of kettle.

Table S2. Quantifier and qualifier ions used in the selected-ion monitoring of the studied analytes by gas chromatography-mass spectrometry (GC-MS)

Compound name	Retention time (min)	Quantifier ion (<i>m/z</i>)	Qualifier ion (<i>m/z</i>)
Ethyl acetate	3.146	88	70
Diethoxyethane	3.185	103	75
Methanol	3.315	32	31
Isobutanol	8.850	43	74
Isoamyl acetate	9.842	70	87
Ethyl hexanoate	13.793	88	99
Ethyl octanoate	20.575	88	127
Furfural	21.504	96	95
Acetic acid	21.661	60	45
Methyl decanoate*	25.009	155	143
2-Phenylethanol	27.510	122	92

*Internal standard

Table S3: Summary of regression data of target analytes

Compound name	Model type	Formula	Origin	Weight	<i>r</i>
Ethyl acetate	Linear	$y = 0.119057 * x - 0.027489$	Include	$1/x^2$	0.9993
Diethoxyethane	Linear	$y = 0.932070 * x + 0.026418$	Ignore	$1/x^2$	0.9996
Methanol	Linear	$y = 0.056843 * x - 0.001007$	Include	None	0.9980
Isobutanol	Quadratic	$y = -0.004171 * x^2 + 0.933144 * x - 0.007372$	Include	None	0.9988
Isoamyl acetate	RF	$y = 2.496215 * x$	Forced	None	0.9995
Ethyl hexanoate	RF	$y = 3.077703 * x$	Forced	None	1.0000
Ethyl octanoate	Linear	$y = 4.887226 * x - 0.004797$	Include	None	0.9996
Furfural	Linear	$y = 2.015309 * x - 0.008687$	Ignore	None	0.9999
Acetic acid	Linear	$y = 0.380350 * x - 0.031256$	Ignore	None	0.9994
2-Phenylethanol	Linear	$y = 1.531632 * x - 0.029097$	Ignore	None	0.9999

*RF: Average Response Factor

Table S4. Congener concentrations (mM) in different fractions from 5-gallon Vevor still, as determined by ¹H NMR. (nd – not detected)

Run #1	1	2	3	4	5	6	7	8	9	10
1-Propanol	3.6	6.2	9.1	9.8	8.4	7.6	6.9	6.0	5.4	4.3
2-Methylbutanol	0.59	1.9	2.8	2.4	1.6	1.5	0.87	0.52	0.36	0.20
2-Phenylethanol	nd	nd	0.0066	0.013	0.023	0.040	0.048	0.050	0.065	0.069
3-Methylbutanol	3.1	6.1	9.7	9.6	6.0	4.7	3.5	2.6	1.7	1.1
Acetaldehyde	29	15	9.3	6.5	4.3	2.8	1.7	1.1	0.70	0.43
Acetic acid	0.10	0.22	0.39	0.46	0.49	0.54	0.67	0.71	0.65	0.87
Ethyl acetate	6.7	3.7	1.7	0.89	0.47	0.27	0.22	0.18	0.17	0.15
Furfural	nd	nd	nd	nd	nd	0.015	0.023	0.025	0.035	0.036
Isobutanol	1.7	3.0	3.8	3.6	2.5	2.0	1.5	1.0	0.76	0.52
Methanol	0.36	0.34	0.31	0.34	0.32	0.36	0.31	0.32	0.33	0.32

Run #2	1	2	3	4	5	6	7	8	9	10
1-Propanol	2.1	2.9	3.6	3.9	2.1	2.7	2.4	2.1	1.7	1.3
2-Methylbutanol	3.9	5.6	6.4	5.5	3.3	2.5	1.9	1.3	0.88	0.46
2-Phenylethanol	0.013	0.026	0.048	0.073	0.30	0.14	0.16	0.19	0.22	0.24
3-Methylbutanol	14	22	29	25	18	13	9.0	6.6	4.3	2.7
Acetaldehyde	14	6.6	4.3	3.2	nd	1.1	0.65	0.41	nd	nd
Acetic acid	nd	0.13	0.22	0.31	1.1	0.53	0.68	0.95	1.1	1.2
Ethyl acetate	11	4.3	1.7	0.89	0.016	0.14	0.066	0.035	0.025	0.017
Furfural	nd	nd	nd	nd	nd	0.004	0.006	0.008	0.009	0.011
Isobutanol	5.6	7.1	7.6	6.4	2.4	3.6	2.5	2.0	1.2	0.80
Methanol	0.36	0.34	0.25	0.40	0.23	0.33	0.27	0.29	0.31	0.34

Run #3	1	2	3	4	5	6	7	8	9	10
1-Propanol	12	17	21	23	23	22	20	17	14	15
2-Methylbutanol	2.7	4.2	5.1	3.7	2.8	2.1	1.6	1.1	0.54	0.78
2-Phenylethanol	0.0052	0.011	0.018	0.034	0.049	0.070	0.077	0.088	0.092	0.089
3-Methylbutanol	9.0	12	14	12	8.9	6.9	5.5	4.0	2.1	3.0
Acetaldehyde	13	6.3	3.8	2.5	1.7	0.95	0.53	0.37	0.12	0.20

Acetic acid	0.072	0.13	0.19	0.22	0.24	0.28	0.29	0.31	0.39	0.35
Ethyl acetate	23	10	4.4	1.9	0.80	0.33	0.12	0.046	0.015	0.021
Furfural	nd	nd	nd	nd	nd	nd	nd	0.0096	0.016	0.011
Isobutanol	5.6	6.7	6.5	5.4	4.3	3.5	2.8	2.2	1.2	1.6
Methanol	0.55	0.51	0.44	0.35	0.33	0.29	0.30	0.30	0.30	0.30

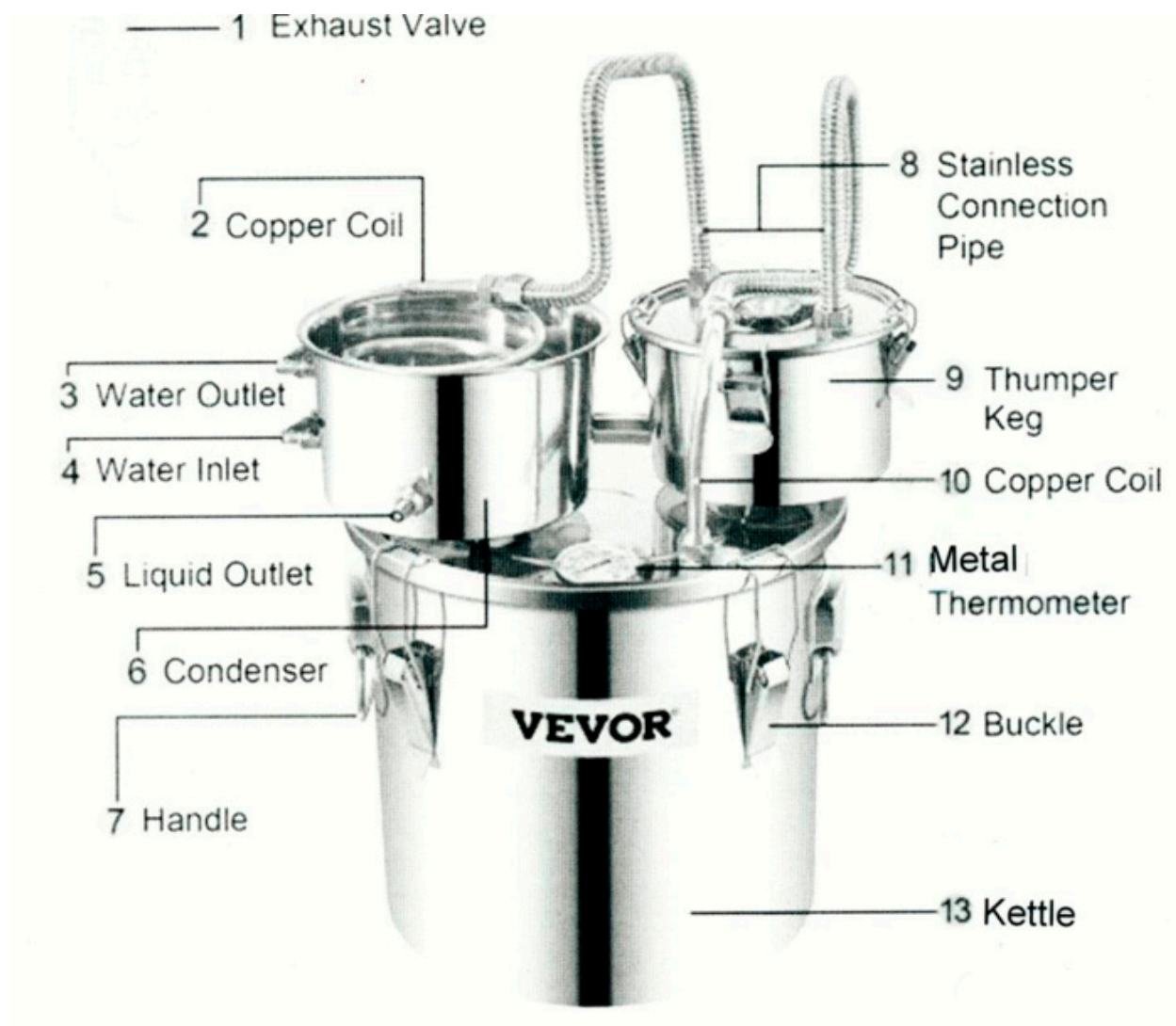


Figure S1. Labeled photograph of the 5 gallon Vevor still



Figure S2. Configuration of the home still in our laboratory.



Figure S3. Distiller's beer in Vevor kettle.

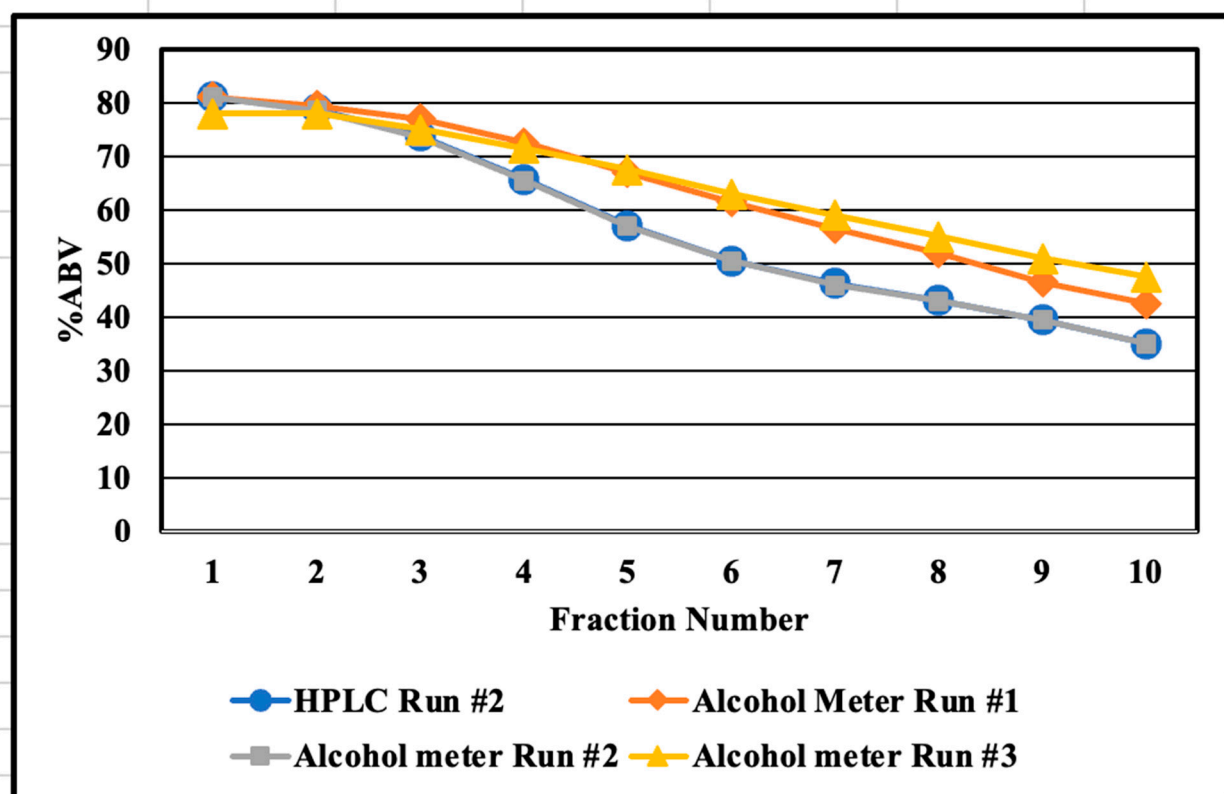


Figure S4. Plot of %ABV versus fraction number for the three runs using alcohol meter data from Table S1 and data obtained with HPLC for Run #2. The data points for Run #2 (alcohol meter) were made smaller so that the data points for Run #2 (HPLC) could be visualized.