Supplementary Materials for Predicting the Physical Properties of Three-Component Lignocellulose Derived Advanced Biofuel Blends Using a Design of Experiments Approach

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S1 Predictions of Other Properties

S1.1 Calculated Property Values

Table S1.1.1. Lower Heating Value (LHV) and Oxygen Content of Different Blend Components.

Fuel Component	LHV (MJ/kg)[a]	Oxygen Content (%)
EN 590 Limits[1]	None specified	None specified
BS 2869 Limits[2]	None specified	None specified
Diesel	42.7	3.0
EL	24.8	33.3
nBL	27.4	27.9
DEE	33.9	21.6
DNBE	38.3	12.3
EtOH	26.8	34.7
nBuOH	33.1	21.6

[a]from[3-7]

Table S1.1.2. Predicted Lower Heating Values using Linear-by-Mass Blending Law and Oxygen Content Predicted using a Linear Blending Law.

Fuel Blend Composition (vol%)	Calculated LHV (MJ/kg)	Oxygen Content (%)
D0Et100 – 80:5:15	25.5	33.1
D0Et100 – 50:40:10	27.7	28.6
D75Et25 – 50:45:5	38.9	9.2
D0Bu100 – 80:5:15	28.6	25.9
D0Bu100 – 50:40:10	31.8	21.4
D75Bu25 – 50:45:5	39.9	7.4

S1.2 Diesel Thermogravimetric Analysis

The diesel was analysed using a Mettler Toledo TGA/DSC 3+, using an alumina crucible with a pierced lid to build up vapour pressure, under a nitrogen atmosphere. The heating rate used was 10 °C/min.

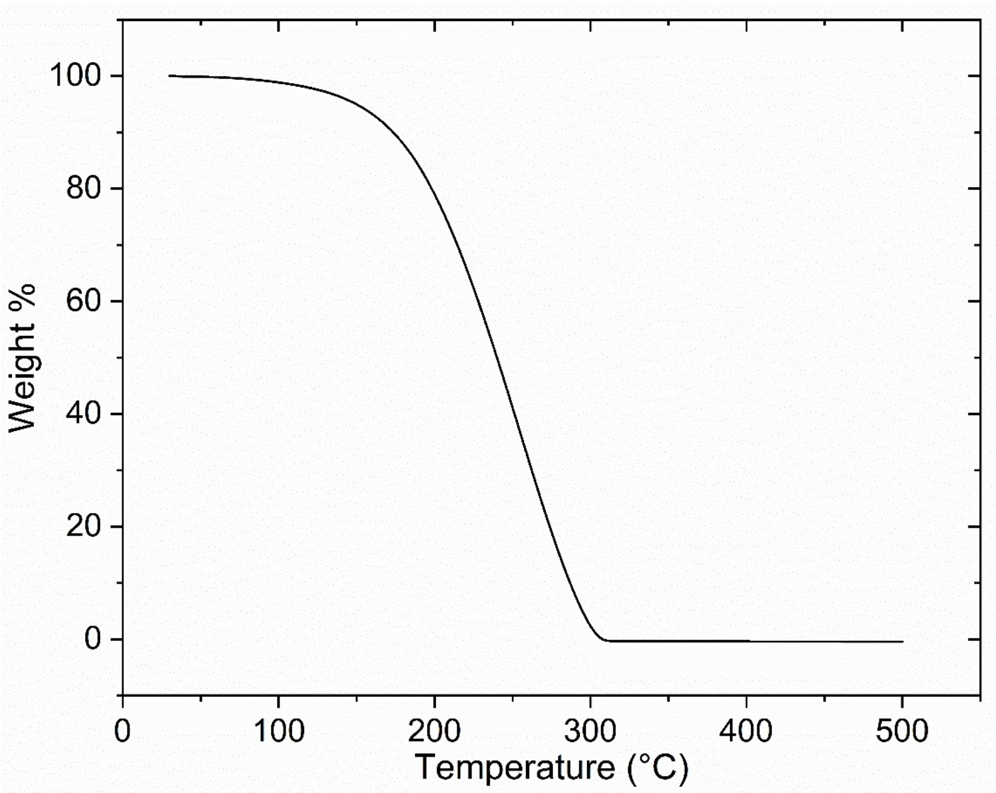

Figure S1. Diesel TGA curve.

Table S1.2.1 Temperatures for given mass fractions remaining from the TGA analysis of the ULSD.

Mass Remaining (%)	Temperature (°C)
99.5	78
95	150
90	173
85	188
80	198
75	207
70	215
65	222
60	228
55	234
50	240
45	246
40	251
35	257
30	262
25	268
20	274
15	280
10	287
5	295
0.5	305

The tables below show the different model coefficients determined by MODDE for the linear, quadratic, and cubic models for predicting the density at 15 °C of the different blends tested.

S2 Density Model Coefficients

S2.1 Ethyl-Based Blends

Table S2.1.1. Linear Model Coefficients for Density Predictions of Ethyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.924	0.002	0.00	0.005
EtOH	-0.133	0.004	1.45×10^{-25}	0.008
EL	0.093	0.003	1.26×10^{-25}	0.005
DEE	-0.189	0.004	4.93×10^{-30}	0.008

The R^2 value of the model was 0.996.

Table S2.1.2. Quadratic Model Coefficients for Density Predictions of Ethyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.921	0.004	0.00	0.009
EtOH	-0.127	0.009	1.88×10^{-13}	0.019
EL	0.086	0.005	8.68×10^{-15}	0.011
DEE	-0.172	0.010	1.09×10^{-15}	0.021
EtOH²	0.052	0.035	1.44×10^{-1}	0.072
EL²	0.024	0.008	4.86×10^{-3}	0.016
DEE²	0.061	0.034	7.95×10^{-2}	0.069
EtOH×EL	-0.081	0.031	1.64×10^{-2}	0.065
EtOH×DEE	0.174	0.068	1.67×10^{-2}	0.139
EL×DEE	-0.086	0.028	4.91×10^{-3}	0.057

The R^2 value of the model was 0.990, which is lower than the R^2 of the linear model. In addition the $EtOH^2$ term is insignificant as it has a p-value above the 0.05 threshold. Removal of this would remove all the EtOH interaction terms due to the model hierarchy and would result in the linear model being reproduced after all of the resultant insignificant terms were removed.

S2.2 Butyl-Based Blends Density Models

Table S2.2.1. Linear Model Coefficients for Density Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.908	0.004	0.00	0.008
nBuOH	-0.112	0.007	2.30×10^{-16}	0.013
nBL	0.070	0.005	3.54×10^{-15}	0.009
DNBE	-0.128	0.006	4.04×10^{-18}	0.013

The R^2 value of the model was 0.977 and all terms are statistically significant.

Table S2.2.2 Quadratic Model Coefficients for Density Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.906	0.003	0.00	0.006
nBuOH	-0.098	0.006	1.35×10^{-14}	0.013
nBL	0.067	0.004	4.81×10^{-16}	0.007
DNBE	-0.133	0.007	6.41×10^{-17}	0.014
nBuOH²	0.043	0.023	7.48×10^{-2}	0.048
nBL²	0.013	0.005	1.58×10^{-2}	0.011
DNBE²	0.053	0.023	2.74×10^{-2}	0.047
nBuOH×nBL	-0.043	0.021	4.76×10^{-2}	0.043
nBuOH×DNBE	0.063	0.045	1.71×10^{-1}	0.092
nBL×DNBE	-0.049	0.019	1.44×10^{-2}	0.038

The R^2 value of the model was 0.992, although this is higher than the linear model there were insignificant terms. Upon removal of the insignificant terms, starting with the nBuOH×DNBE term this resulted in the other quadratic terms becoming insignificant, resulting in the linear model.

S2.3 Pentyl Based Blends Density Models

Table S2.3.1 Linear Model Coefficients for Density Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.906	0.001	0.00	0.002
nPeOH	-0.090	0.001	5.63×10^{-33}	0.003
nPL	0.060	0.001	3.39×10^{-32}	0.002
DNPE	-0.117	0.001	1.30×10^{-36}	0.003

The R^2 value of the model was 0.998 and all terms are significant.

Table S2.3.2 Quadratic Model Coefficients for Density Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	0.905	0.001	0.00	0.003
nPeOH	-0.088	0.003	1.13×10^{-21}	0.006
nPL	0.058	0.002	7.41×10^{-23}	0.004
DNPE	-0.114	0.003	5.52×10^{-24}	0.007
nPeOH²	0.030	0.012	1.56×10^{-2}	0.024
nPL²	0.008	0.003	4.69×10^{-3}	0.005
DNPE²	0.030	0.011	1.37×10^{-2}	0.024
nPeOH×nPL	-0.027	0.010	1.30×10^{-2}	0.021
nPeOH×DNPE	0.033	0.021	1.36×10^{-1}	0.044
nPL×DNPE	-0.027	0.009	6.91×10^{-3}	0.019

The R^2 value of the model was 0.997.

The nPeOH×DNPE term was insignificant with a p-value >0.05. Upon removal of this term, it generated other insignificant terms, ultimately resulting in the linear model.

S3 Flash Point Coefficients

S3.1 Butyl-Based Blends Flash Model Coefficients

Table S3.1.1. Linear Model Coefficients for Flash Point Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	37.342	3.556	4.19×10^{-9}	7.471
nBuOH	-22.885	6.386	2.12×10^{-3}	13.417
nBL	18.726	4.133	2.59×10^{-4}	8.683
DNBE	-41.805	6.265	2.93×10^{-6}	13.163

The R^2 value of the model was 0.813, indicating it may not be that accurate at predicting the flash points of the blends.

Table S3.1.2. Quadratic Model Coefficients for Flash Point Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	34.930	2.268	1.38×10^{-14}	4.66128
nBuOH	-7.989	4.856	1.12×10^{-1}	9.98254
nBL	8.066	2.903	1.00×10^{-2}	5.96782
DNBE	-19.876	5.292	8.80×10^{-4}	10.8769
$nBuOH^2$	82.012	18.411	1.42×10^{-4}	37.8448
nBL^2	26.872	4.135	6.90×10^{-7}	8.50037
$DNBE^2$	54.242	17.801	5.25×10^{-3}	36.5907
nBuOH×nBL	-100.870	16.602	2.03×10^{-6}	34.1255
nBuOH×DNBE	184.435	35.841	2.29×10^{-5}	73.6715
nBL×DNBE	-84.792	14.750	4.72×10^{-6}	30.3179

The R^2 value of the model was R^2 0.924. The insignificance of the nBuOH term was discussed in section Flash Points section.

S3.2 Pentyl-Based Blends Flash Point Model Coefficients

Table S3.2.1 Linear Model Coefficients for Flash Point Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	61.775	2.614	0.00	5.338
nPeOH	-41.346	4.057	0.00	8.285
nPL	16.683	2.872	0.00	5.865
DNPE	-16.286	3.989	3.00×10^{-4}	8.147

The R^2 value of the model was 0.870, indicating it may not be that accurate at predicting the flash points of the blends.

Table S3.2.2 Quadratic Model Coefficients for Flash Point Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	58.956	1.099	5.69×10^{-29}	2.255
nPeOH	-42.840	2.332	8.67×10^{-17}	4.785
nPL	14.790	1.394	3.93×10^{-11}	2.860
DNPE	-8.254	2.460	2.36×10^{-3}	5.047
nPeOH²	103.317	8.888	5.12×10^{-12}	18.237
nPL²	15.329	1.920	1.40×10^{-8}	3.939
DNPE²	31.103	8.663	1.29×10^{-3}	17.774
nPeOH×nPL	-73.858	7.694	3.38×10^{-10}	15.786
nPeOH×DNPE	48.514	16.176	5.76×10^{-3}	33.190
nPL×DNPE	-32.051	6.981	9.14×10^{-5}	14.325

The R^2 value of the model was 0.982.

S4 KV40 Model Coefficients

S4.1 Butyl-Based Blends KV40 Model Coefficients

Table S4.1.1. Linear Model Coefficients for KV40 Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	1.509	0.030	5.13×10^{-29}	0.061
nBuOH	-0.172	0.048	1.17×10^{-3}	0.097
nBL	0.378	0.033	4.19×10^{-12}	0.067
DNBE	-1.133	0.047	2.32×10^{-20}	0.096

The R^2 value of the model was 0.973.

Table S4.1.2. Quadratic Model Coefficients for KV40 Predictions of Butyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	1.469	0.033	2.75×10^{-25}	0.068
nBuOH	-0.163	0.072	3.37×10^{-2}	0.149
nBL	0.317	0.043	8.39×10^{-8}	0.088
DNBE	-0.932	0.077	6.62×10^{-12}	0.159
nBuOH²	1.596	0.273	4.25×10^{-6}	0.562
nBL²	0.264	0.060	1.94×10^{-4}	0.124
DNBE²	0.309	0.265	2.54×10^{-1}	0.545
nBuOH×nBL	-1.284	0.244	1.88×10^{-5}	0.502
nBuOH×DNBE	1.242	0.524	2.58×10^{-2}	1.079
nBL×DNBE	-0.538	0.218	2.05×10^{-2}	0.448

The R^2 value of the model was 0.975. The removal of the insignificant terms reduced the model to an inaccurate model.

S4.2 Pentyl-Based Blends KV40 Model Coefficients

Table S4.2.1 Linear Model Coefficients for KV40 Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	1.866	0.031	1.15×10^{-32}	0.064
nPeOH	-0.155	0.049	3.44×10^{-3}	0.100
nPL	0.358	0.035	2.02×10^{-11}	0.071
DNPE	-1.080	0.048	2.39×10^{-20}	0.098

The R^2 value of the model was 0.967.

Table S4.2.2. Quadratic Model Coefficients for KV40 Predictions of Pentyl-Based Blends

	Coefficient	Standard Error	P-Value	95% Confidence interval (±)
Constant	1.831	0.008	0.00	0.017
nPeOH	-0.196	0.018	1.63×10^{-11}	0.036
nPL	0.339	0.011	5.01×10^{-23}	0.022
DNPE	-0.977	0.019	1.13×10^{-28}	0.038
$nPeOH^2$	1.363	0.068	8.03×10^{-18}	0.139
nPL^2	0.178	0.015	1.67×10^{-12}	0.030
$DNPE^2$	0.288	0.066	1.59×10^{-4}	0.135
nPeOH×nPL	-0.926	0.058	3.38×10^{-15}	0.120
nPeOH×DNPE	0.473	0.123	6.53×10^{-4}	0.252
nPL×DNPE	-0.304	0.053	4.29×10^{-6}	0.109

The R^2 value of the model was 0.998. All terms were statistically significant.

S5 Experimental Data

All the errors reported for the measured density, flash points, and KV40 are the standard deviations of three repeated measurements. The errors reported for the predicted values are the model's 95% confidence intervals.

S5.1 Ethyl-Based Three-Component Blends

Table S5.1.1. Measured and Predicted Density of the Ethyl-Based Blends.

Data Use	EL (vol%)	DEE (vol%)	EtOH (vol%)	Measured Density (g/cm³)	Predicted Density (g/cm³)
MODDE Generated blends	0.5	0.05	0.45	0.899 ± 0.002	0.901 ± 0.002
	0.7	0.05	0.25	0.945 ± 0.001	0.946 ± 0.001
	0.75	0.1	0.15	0.954 ± 0.001	0.955 ± 0.001
	0.55	0.1	0.35	0.910 ± 0.002	0.909 ± 0.002
	0.6	0.2	0.2	0.915 ± 0.001	0.915 ± 0.001
	0.6	0.2	0.2	0.918 ± 0.001	0.915 ± 0.001
	0.5	0.25	0.25	0.891 ± 0.001	0.890 ± 0.001
	0.6	0.2	0.2	0.916 ± 0.001	0.915 ± 0.001
	0.55	0.3	0.15	0.899 ± 0.002	0.898 ± 0.001
	0.5	0.45	0.05	0.879 ± 0.003	0.878 ± 0.002
	0.9	0.05	0.05	0.989 ± 0.001	0.991 ± 0.002
	0.7	0.25	0.05	0.936 ± 0.001	0.935 ± 0.001
	0.5	0.05	0.45	0.901 ± 0.001	0.901 ± 0.002
	0.5	0.45	0.05	0.876 ± 0.001	0.878 ± 0.002
	0.9	0.05	0.05	0.987 ± 0.001	0.991 ± 0.002
	0.633	0.317	0.05	0.916 ± 0.001	0.916 ± 0.001
	0.767	0.183	0.05	0.949 ± 0.001	0.954 ± 0.001
	0.5	0.317	0.183	0.887 ± 0.002	0.886 ± 0.001
	0.767	0.05	0.183	0.959 ± 0.001	0.961 ± 0.001
	0.633	0.183	0.183	0.919 ± 0.001	0.924 ± 0.001
	0.633	0.183	0.183	0.925 ± 0.001	0.924 ± 0.001
Blends added for increased coverage	0.8	0.15	0.05	0.963 ± 0.001	0.963 ± 0.001
	0.5	0.4	0.1	0.880 ± 0.001	0.881 ± 0.002
	0.5	0.1	0.4	0.897 ± 0.002	0.898 ± 0.002
	0.75	0.2	0.05	0.948 ± 0.001	0.949 ± 0.001
	0.55	0.35	0.1	0.895 ± 0.002	0.895 ± 0.001
	0.6	0.15	0.25	0.918 ± 0.001	0.918 ± 0.001
	0.8	0.15	0.05	0.966 ± 0.001	0.963 ± 0.001
	0.8	0.1	0.1	0.970 ± 0.001	0.966 ± 0.001
	0.8	0.05	0.15	0.973 ± 0.001	0.969 ± 0.001
	0.85	0.1	0.05	0.981 ± 0.001	0.977 ± 0.001
	0.85	0.05	0.1	0.983 ± 0.001	0.980 ± 0.002
Model Validation	0.55	0.2	0.25	0.908 ± 0.001	0.904 ± 0.001
	0.6	0.25	0.15	0.918 ± 0.001	0.912 ± 0.001
	0.65	0.25	0.1	0.930 ± 0.001	0.924 ± 0.001
	0.65	0.1	0.25	0.937 ± 0.001	0.932 ± 0.001
	0.7	0.2	0.1	0.943 ± 0.002	0.938 ± 0.001
	0.7	0.15	0.15	0.945 ± 0.001	0.941 ± 0.001

S5.2 Butyl-Based Three-Component Blends

Table S5.2.2. Measured and Predicted Properties of the Butyl-Based Blends.

	nBL (vol%)	DNBE (vol%)	nBuOH (vol%)	Measured Density (g/cm³)	Predicted Density (g/cm³)	Measured Flash Point (°C)	Predicted Flash Point (°C)	Measured KV40 (mm²/s)	Predicted KV40 (mm²/s)
MODDE Generated blends	0.7	0.05	0.25	0.926 ± 0.001	0.922 ± 0.002	41.3 ± 0.6	37.78 ± 2.34	1.636 ± 0.001	1.605 ± 0.034
	0.5	0.25	0.25	0.882 ± 0.001	0.882 ± 0.002	30.5 ± 1.3	35.39 ± 2.33	1.395 ± 0.001	1.389 ± 0.034
	0.5	0.45	0.05	0.875 ± 0.001	0.879 ± 0.004	26.3 ± 1.5	30.16 ± 2.59	1.186 ± 0.001	1.207 ± 0.038
	0.6	0.2	0.2	0.902 ± 0.001	0.901 ± 0.002	33.0 ± 1.0	34.32 ± 1.31	1.467 ± 0.001	1.442 ± 0.019
	0.55	0.3	0.15	0.890 ± 0.001	0.890 ± 0.002	31.0 ± 1.4	32.93 ± 1.36	1.326 ± 0.001	1.344 ± 0.020
	0.75	0.1	0.15	0.928 ± 0.001	0.930 ± 0.002	42.7 ± 0.6	40.32 ± 1.35	1.608 ± 0.001	1.610 ± 0.020
	0.7	0.25	0.05	0.918 ± 0.001	0.919 ± 0.002	37.3 ± 1.0	35.87 ± 1.98	1.455 ± 0.001	1.479 ± 0.029
	0.9	0.05	0.05	0.956 ± 0.001	0.958 ± 0.003	57.0 ± 0.0	54.93 ± 2.37	1.804 ± 0.001	1.839 ± 0.035
	0.55	0.1	0.35	0.895 ± 0.001	0.894 ± 0.003	33.7 ± 0.6	35.74 ± 1.45	1.553 ± 0.001	1.538 ± 0.021
	0.5	0.05	0.45	0.889 ± 0.001	0.885 ± 0.004	38.3 ± 0.6	37.43 ± 2.62	1.611 ± 0.001	1.623 ± 0.038
	0.6	0.2	0.2	0.897 ± 0.001	0.901 ± 0.002	36.0 ± 0.0	34.32 ± 1.31	1.439 ± 0.001	1.442 ± 0.019
	0.6	0.2	0.2	0.902 ± 0.001	0.901 ± 0.002	35.5 ± 0.6	34.32 ± 1.31	1.472 ± 0.001	1.442 ± 0.019
	0.5	0.45	0.05	0.874 ± 0.001	0.879 ± 0.004	32.0 ± 0.0	30.16 ± 2.59	1.214 ± 0.001	1.207 ± 0.038
	0.9	0.05	0.05	0.957 ± 0.001	0.958 ± 0.003	53.7 ± 0.6	54.93 ± 2.37	1.846 ± 0.001	1.839 ± 0.035
	0.5	0.05	0.45	0.891 ± 0.001	0.885 ± 0.004	37.0 ± 0.0	37.43 ± 2.62	1.585 ± 0.001	1.623 ± 0.038
	0.633	0.317	0.05	0.901 ± 0.001	0.905 ± 0.002	34.7 ± 0.6	32.47 ± 1.94	1.406 ± 0.001	1.378 ± 0.028
	0.767	0.183	0.05	0.928 ± 0.001	0.932 ± 0.002	41.0 ± 0.0	40.77 ± 1.75	1.624 ± 0.001	1.589 ± 0.025
	0.5	0.317	0.183	0.879 ± 0.001	0.881 ± 0.002	33.0 ± 0.0	33.99 ± 2.09	1.287 ± 0.001	1.322 ± 0.030
	0.767	0.05	0.183	0.936 ± 0.001	0.934 ± 0.002	43.7 ± 0.6	41.65 ± 2.03	1.693 ± 0.001	1.656 ± 0.029
	0.633	0.183	0.183	0.907 ± 0.001	0.908 ± 0.002	35.0 ± 0.0	34.85 ± 1.28	1.471 ± 0.001	1.469 ± 0.019
	0.633	0.183	0.183	0.908 ± 0.001	0.908 ± 0.002	34.8 ± 0.8	34.85 ± 1.28	1.555 ± 0.001	1.469 ± 0.019
Blends added for increased coverage	0.8	0.1	0.1	0.939 ± 0.001	0.939 ± 0.002	44.0 ± 1.4	44.09 ± 1.16	1.671 ± 0.001	1.668 ± 0.017
	0.8	0.05	0.15	0.941 ± 0.001	0.940 ± 0.002	45.0 ± 0.0	44.25 ± 1.80	1.697 ± 0.001	1.691 ± 0.026
	0.85	0.1	0.05	0.951 ± 0.001	0.948 ± 0.003	46.0 ± 1.0	48.91 ± 1.66	1.711 ± 0.001	1.741 ± 0.024
	0.85	0.05	0.1	0.952 ± 0.001	0.949 ± 0.003	48.5 ± 0.7	49.07 ± 1.69	1.750 ± 0.001	1.757 ± 0.025
	0.8	0.15	0.05	0.938 ± 0.001	0.938 ± 0.002	42.5 ± 0.8	43.73 ± 1.61	1.641 ± 0.001	1.648 ± 0.023
	0.5	0.4	0.1	0.878 ± 0.001	0.880 ± 0.003	31.7 ± 0.6	31.77 ± 1.85	1.220 ± 0.001	1.248 ± 0.027
	0.5	0.1	0.4	0.891 ± 0.001	0.885 ± 0.003	37.0 ± 0.0	37.22 ± 1.98	1.520 ± 0.001	1.560 ± 0.029
	0.75	0.2	0.05	0.927 ± 0.001	0.928 ± 0.002	38.7 ± 0.6	39.38 ± 1.83	1.558 ± 0.001	1.560 ± 0.027

	0.55	0.35	0.1	0.889 ± 0.001	0.890 ± 0.003	33.0 ± 0.0	31.73 ± 1.32	1.286 ± 0.001	1.304 ± 0.019
	0.6	0.15	0.25	0.905 ± 0.001	0.902 ± 0.002	36.0 ± 0.0	34.91 ± 1.32	1.490 ± 0.001	1.486 ± 0.019
Model Validation	0.55	0.2	0.25	0.895 ± 0.001	0.892 ± 0.002	34.0 ± 0.0	34.73 ± 1.58	1.416 ± 0.001	1.435 ± 0.023
	0.6	0.25	0.15	0.902 ± 0.001	0.900 ± 0.002	34.0 ± 0.0	33.53 ± 1.25	1.422 ± 0.001	1.402 ± 0.018
	0.65	0.25	0.1	0.911 ± 0.001	0.909 ± 0.002	35.7 ± 0.6	34.17 ± 1.43	1.422 ± 0.001	1.433 ± 0.021
	0.65	0.1	0.25	0.915 ± 0.001	0.912 ± 0.002	38.7 ± 0.6	35.93 ± 1.64	1.554 ± 0.001	1.543 ± 0.024
	0.7	0.2	0.1	0.920 ± 0.001	0.919 ± 0.002	36.3 ± 0.6	36.64 ± 1.41	1.498 ± 0.001	1.505 ± 0.020
	0.7	0.15	0.15	0.923 ± 0.001	0.920 ± 0.002	36.7 ± 0.6	37.22 ± 1.27	1.543 ± 0.001	1.535 ± 0.018

S5.3 Pentyl-Based Three-Component Blends

Table S5.3.1. Measured and Predicted Properties of the Pentyl-Based Blends.

	nPL (vol%)	DNPE (vol%)	nPeOH (vol%)	Measured Density (g/cm³)	Predicted Density (g/cm³)	Measured Flash Point (°C)	Predicted Flash Point (°C)	Measured KV40 (mm²/s)	Predicted KV40 (mm²/s)
MODDE Generated blends	0.7	0.05	0.25	0.920 ± 0.001	0.919 ± 0.001	59.7 ± 0.6	58.79 ± 1.03	1.977 ± 0.001	1.977 ± 0.008
	0.5	0.25	0.25	0.884 ± 0.001	0.884 ± 0.001	55.7 ± 0.6	55.61 ± 1.10	1.732 ± 0.001	1.731 ± 0.008
	0.5	0.45	0.05	0.879 ± 0.001	0.879 ± 0.001	63.7 ± 0.6	62.92 ± 1.21	1.577 ± 0.001	1.577 ± 0.009
	0.6	0.2	0.2	0.900 ± 0.001	0.900 ± 0.001	58.0 ± 0.0	57.74 ± 0.63	1.815 ± 0.001	1.801 ± 0.005
	0.55	0.3	0.15	0.890 ± 0.001	0.890 ± 0.001	58.7 ± 0.6	58.75 ± 0.65	1.712 ± 0.001	1.700 ± 0.005
	0.75	0.1	0.15	0.924 ± 0.001	0.925 ± 0.001	63.0 ± 0.0	64.07 ± 0.62	1.981 ± 0.001	1.972 ± 0.005
	0.7	0.25	0.05	0.914 ± 0.001	0.914 ± 0.001	66.3 ± 0.6	67.23 ± 0.89	1.844 ± 0.001	1.843 ± 0.007
	0.9	0.05	0.05	0.950 ± 0.001	0.949 ± 0.001	76.7 ± 0.6	77.82 ± 1.12	2.180 ± 0.001	2.172 ± 0.009
	0.55	0.1	0.35	0.895 ± 0.001	0.896 ± 0.001	55.3 ± 0.6	54.59 ± 0.66	1.902 ± 0.001	1.897 ± 0.005
	0.5	0.05	0.45	0.890 ± 0.001	0.889 ± 0.001	54.3 ± 0.6	55.16 ± 1.22	1.975 ± 0.001	1.980 ± 0.009
	0.6	0.2	0.2	0.900 ± 0.001	0.900 ± 0.001	58.7 ± 0.6	57.74 ± 0.63	1.799 ± 0.001	1.801 ± 0.005
	0.6	0.2	0.2	0.896 ± 0.001	0.900 ± 0.001	58.7 ± 0.6	57.74 ± 0.63	1.777 ± 0.001	1.801 ± 0.005
	0.5	0.45	0.05	0.878 ± 0.001	0.879 ± 0.001	63.0 ± 0.0	62.92 ± 1.21	1.578 ± 0.001	1.577 ± 0.009
	0.9	0.05	0.05	0.949 ± 0.001	0.949 ± 0.001	80.7 ± 0.6	77.82 ± 1.12	2.171 ± 0.001	2.172 ± 0.009
	0.5	0.05	0.45	0.889 ± 0.001	0.889 ± 0.001	54.7 ± 0.6	55.16 ± 1.22	1.982 ± 0.001	1.980 ± 0.009
	0.633	0.317	0.05	0.902 ± 0.001	0.902 ± 0.001	66.0 ± 0.0	65.09 ± 0.86	1.752 ± 0.001	1.747 ± 0.007
	0.767	0.183	0.05	0.926 ± 0.001	0.926 ± 0.001	71.0 ± 0.0	70.08 ± 0.81	1.946 ± 0.001	1.946 ± 0.006
	0.5	0.317	0.183	0.883 ± 0.001	0.882 ± 0.001	56.7 ± 0.6	57.29 ± 0.99	1.665 ± 0.001	1.669 ± 0.008
	0.767	0.05	0.183	0.930 ± 0.001	0.929 ± 0.001	62.0 ± 0.0	63.45 ± 0.91	2.017 ± 0.001	2.020 ± 0.007

	0.633	0.183	0.183	0.907 ± 0.001	0.906 ± 0.001	58.7 ± 0.6	58.96 ± 0.61	1.833 ± 0.001	1.831 ± 0.005
	0.633	0.183	0.183	0.906 ± 0.001	0.906 ± 0.001	58.7 ± 0.6	58.96 ± 0.61	1.835 ± 0.001	1.831 ± 0.005
Blends added for increased coverage	0.8	0.15	0.05	0.932 ± 0.001	0.932 ± 0.001	71.3 ± 0.6	71.74 ± 0.75	2.003 ± 0.001	2.000 ± 0.006
	0.5	0.4	0.1	0.880 ± 0.001	0.880 ± 0.001	59.3 ± 0.6	60.45 ± 0.88	1.602 ± 0.001	1.606 ± 0.007
	0.5	0.1	0.4	0.889 ± 0.001	0.888 ± 0.001	55.0 ± 0.0	54.63 ± 0.94	1.907 ± 0.001	1.909 ± 0.007
	0.75	0.2	0.05	0.923 ± 0.001	0.923 ± 0.001	69.0 ± 0.0	69.29 ± 0.84	1.911 ± 0.001	1.920 ± 0.006
	0.55	0.35	0.1	0.889 ± 0.001	0.889 ± 0.001	60.3 ± 0.6	60.86 ± 0.61	1.666 ± 0.001	1.666 ± 0.005
	0.6	0.15	0.25	0.903 ± 0.001	0.902 ± 0.001	57.0 ± 0.0	56.41 ± 0.62	1.850 ± 0.001	1.846 ± 0.005
	0.6	0.35	0.05	0.896 ± 0.001	0.896 ± 0.001	64.7 ± 0.6	64.29 ± 0.83	1.696 ± 0.001	1.702 ± 0.006
	0.6	0.05	0.35	0.905 ± 0.001	0.904 ± 0.001	55.7 ± 0.6	55.05 ± 0.93	1.954 ± 0.001	1.954 ± 0.007
	0.8	0.1	0.1	0.933 ± 0.001	0.933 ± 0.001	67.0 ± 0.0	68.85 ± 0.55	2.009 ± 0.001	2.022 ± 0.004
	0.8	0.05	0.15	0.935 ± 0.001	0.934 ± 0.001	66.7 ± 0.6	66.38 ± 0.83	2.055 ± 0.001	2.050 ± 0.006
	0.85	0.1	0.05	0.941 ± 0.001	0.940 ± 0.001	75.0 ± 0.0	74.58 ± 0.79	2.083 ± 0.001	2.084 ± 0.006
	0.85	0.05	0.1	0.941 ± 0.001	0.942 ± 0.001	71.0 ± 0.0	71.62 ± 0.80	2.098 ± 0.001	2.105 ± 0.006
Model Validation	0.55	0.2	0.25	0.893 ± 0.001	0.893 ± 0.001	55.0 ± 0.0	55.81 ± 0.75	1.914 ± 0.001	1.787 ± 0.006
	0.6	0.25	0.15	0.897 ± 0.001	0.899 ± 0.001	58.7 ± 0.6	59.49 ± 0.59	1.754 ± 0.001	1.762 ± 0.005
	0.65	0.25	0.1	0.906 ± 0.001	0.906 ± 0.001	62.0 ± 0.0	62.88 ± 0.65	1.798 ± 0.001	1.797 ± 0.005
	0.65	0.1	0.25	0.911 ± 0.001	0.910 ± 0.001	58.0 ± 0.0	57.41 ± 0.73	1.917 ± 0.001	1.910 ± 0.006
	0.7	0.2	0.1	0.915 ± 0.001	0.915 ± 0.001	63.0 ± 0.0	64.48 ± 0.65	1.874 ± 0.001	1.868 ± 0.005
	0.7	0.15	0.15	0.917 ± 0.001	0.917 ± 0.001	61.0 ± 0.0	62.15 ± 0.59	1.914 ± 0.001	1.898 ± 0.004

S5.4 Butyl-Based Blends with ULSD

Table S.5.4.1. Measured Properties of the Butyl-Based Blends with ULSD.

ULSD (vol%)	Biofuel Fraction (vol%)	nBL (vol%)	DNBE (vol%)	nBuOH (vol%)	Measured Density (g/cm³)	Measured Flash Point (°C)	KV40 (mm²/s)
100	0	0	0	0	0.840 ± 0.001	65.0 ± 0.0	
95	5	50	45	5	0.842 ± 0.001	58.0 ± 0.8	2.653 ± 0.002
90	10				0.844 ± 0.001	54.3 ± 0.6	2.485 ± 0.001
75	25				0.848 ± 0.001	45.0 ± 1.0	2.109 ± 0.001
50	50				0.857 ± 0.001	41.7 ± 0.6	1.691 ± 0.001
30	70				0.866 ± 0.001	37.0 ± 0.0	1.443 ± 0.001
20	80				0.871 ± 0.001	36.7 ± 0.6	1.347 ± 0.001
0	100				0.875 ± 0.001	32.0 ± 0.0	1.186 ± 0.001

95	5				0.843 ± 0.001	46.7 ± 0.6	2.666 ± 0.001
90	10				0.845 ± 0.001	42.0 ± 0.0	2.536 ± 0.002
75	25				0.852 ± 0.001	40.3 ± 0.6	2.269 ± 0.001
50	50	50	5	45	0.866 ± 0.001	39.7 ± 0.6	1.989 ± 0.001
30	70				0.877 ± 0.001	38.7 ± 0.6	1.807 ± 0.001
20	80				0.882 ± 0.001	38.7 ± 0.6	1.732 ± 0.001
0	100				0.889 ± 0.001	37.7 ± 0.4	1.611 ± 0.001
95	5				0.843 ± 0.001	58.0 ± 1.0	2.552 ± 0.001
90	10				0.845 ± 0.001	53.3 ± 0.6	2.405 ± 0.001
75	25				0.853 ± 0.001	50.0 ± 0.8	2.097 ± 0.001
50	50	60	35	5	0.868 ± 0.001	43.3 ± 0.6	1.761 ± 0.001
30	70				0.881 ± 0.001	41.5 ± 0.6	1.566 ± 0.001
20	80				0.886 ± 0.001	38.7 ± 0.6	1.475 ± 0.001
0	100				0.898 ± 0.001	31.3 ± 1.8	1.329 ± 0.001
95	5				0.844 ± 0.001	47.7 ± 0.6	2.565 ± 0.001
90	10				0.846 ± 0.001	43.7 ± 0.6	2.454 ± 0.001
75	25				0.856 ± 0.001	41.5 ± 0.6	2.217 ± 0.001
50	50	60	5	35	0.877 ± 0.001	41.0 ± 0.0	1.963 ± 0.001
30	70				0.889 ± 0.001	40.3 ± 0.6	1.807 ± 0.001
20	80				0.897 ± 0.001	40.0 ± 0.0	1.733 ± 0.001
0	100				0.911 ± 0.001	35.3 ± 2.1	1.611 ± 0.001
95	5				0.844 ± 0.001	53.8 ± 1.8	2.674 ± 0.001
90	10				0.848 ± 0.001	45.8 ± 0.4	2.519 ± 0.001
75	25				0.859 ± 0.001	41.0 ± 0.0	2.220 ± 0.001
50	50	70	25	5	0.879 ± 0.001	41.7 ± 1.0	1.888 ± 0.001
30	70				0.895 ± 0.001	40.1 ± 0.7	1.685 ± 0.001
20	80				0.902 ± 0.001	38.0 ± 0.0	1.605 ± 0.001
0	100				0.918 ± 0.001	41.3 ± 0.6	1.455 ± 0.001
95	5				0.844 ± 0.001	56.0 ± 0.0	2.582 ± 0.001
90	10				0.848 ± 0.001	55.7 ± 1.2	2.471 ± 0.001
75	25				0.860 ± 0.001	51.4 ± 0.5	2.235 ± 0.001
50	50	70	5	25	0.882 ± 0.001	46.7 ± 0.6	1.988 ± 0.001
30	70				0.899 ± 0.001	42.7 ± 0.6	1.825 ± 0.001
20	80				0.910 ± 0.001	38.0 ± 0.0	1.760 ± 0.001
0	100				0.926 ± 0.001	37.3 ± 1.0	1.636 ± 0.001

95	5				0.845 ± 0.001	58.7 ± 0.6	2.604 ± 0.001
90	10				0.850 ± 0.001	57.0 ± 0.0	2.489 ± 0.001
75	25				0.865 ± 0.001	54.3 ± 0.6	2.244 ± 0.001
50	50	80	15	5	0.889 ± 0.001	51.3 ± 0.6	1.995 ± 0.002
30	70				0.908 ± 0.001	49.0 ± 0.0	1.814 ± 0.001
20	80				0.921 ± 0.001	46.7 ± 0.6	1.765 ± 0.001
0	100				0.938 ± 0.001	44.5 ± 0.7	1.627 ± 0.001
95	5				0.845 ± 0.001	55.7 ± 0.6	2.586 ± 0.002
90	10				0.850 ± 0.001	53.3 ± 0.6	2.481 ± 0.001
75	25				0.865 ± 0.001	48.7 ± 0.6	2.278 ± 0.001
50	50	80	5	15	0.890 ± 0.001	47.3 ± 0.6	2.043 ± 0.001
30	70				0.913 ± 0.001	46.7 ± 0.6	1.893 ± 0.001
20	80				0.923 ± 0.001	43.7 ± 0.6	1.829 ± 0.001
0	100				0.941 ± 0.001	45.0 ± 0.0	1.697 ± 0.001
95	5				0.845 ± 0.001	61.5 ± 0.7	2.603 ± 0.001
90	10				0.851 ± 0.001	59.3 ± 0.6	2.516 ± 0.002
75	25				0.869 ± 0.001	58.3 ± 0.6	2.309 ± 0.002
50	50	90	5	5	0.899 ± 0.001	57.0 ± 0.0	2.114 ± 0.001
30	70				0.923 ± 0.001	57.0 ± 0.0	1.985 ± 0.001
20	80				0.935 ± 0.001	56.7 ± 0.6	1.938 ± 0.001
0	100				0.957 ± 0.001	55.3 ± 0.4	1.804 ± 0.001

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