Supplementary Information (SI) for Sustainable Energy & Fuels.

1. Appendix

1.1. Sulphur measurement

To measure the sulphur concentration using the ICPMS, samples must be diluted following a specific procedure and a calibration curve must be built.

Preparation of samples:

Samples were diluted as follows: 0.5g of biodiesel diluted to 50ml (19.7g) ethanol solution. Further dilution might be required for high S samples to ensure that they are within the calibration range. All samples should have a similar dilution factor since different concentration of organic compounds in the biodiesel might influence how the samples are nebulised in the ICPMS and therefore leading to an error in the results. The dilution solution was made by adding 20ml of nitric acid (HNO3) and 1ml of indium solution into 1000mL of ethanol. This solution will be used for dilution of all samples and calibrations.

Preparation of calibration curve:

Calibration curve was prepared using sulphur-containing biodiesel standards with known concentrations. Each standard is diluted by mixing 1g of biodiesel with 25ml of dilution solution. The concentration of calibration curve for quantification are blank – 0 ppb, 400ppb, 600ppb, 800ppb, 1000ppb, 2000ppb. 4000ppb, 20000ppb.

1.2. Batch result

Table S1: Sulphur content measured by ICP-MS for batch and biodiesel model

Sample	ID	Dilution ratio	IPCMS result (ppb)	S content (ppm)
Sulfolane	Sulf1	2500	7922.72	19806.81
Sulfolane	Sulf2	2500	9020.15	22550.36
Sulfolane	Sulf3	2500	8222.39	20555.98
BMIM AlCl4	AlCl41	100	1682.07	168.21
BMIM AlCl4	AlCl42	100	2046.21	204.62
BMIM AlCl4	AlCl43	100	1269.69	126.97
BMIM MSA	MSA1	2500	237.27	593.19
BMIM MSA	MSA2	2500	213.64	534.11
BMIM MSA	MSA3	2500	152.04	380.09
ChCL:Ph	Ph1	100	3346.55	334.65
ChCL:Ph	Ph2	100	2751.66	275.17
ChCL:Ph	Ph3	100	2944.46	294.45
ChCl:PEG	PEG1	100	2461.01	246.10
ChCl:PEG	PEG2	100	2730.58	273.06
ChCl:PEG	PEG3	100	2840.84	284.08

Biodiesel raw	BR1	25	2116.00	52.90
Biodiesel raw	BR2	25	1956.00	48.90
Biodiesel + 800 S	BS1	25	30194.00	754.85
Biodiesel + 800 S	BS2	25	34920.00	873.00
Biodiesel + 400 S	BSN1	100	3914.67	391.47
Biodiesel + 400 S	BSN2	100	4010.40	401.04
Biodiesel + 400 S	BSN3	100	3903.49	390.35

1.3. Optimisation data

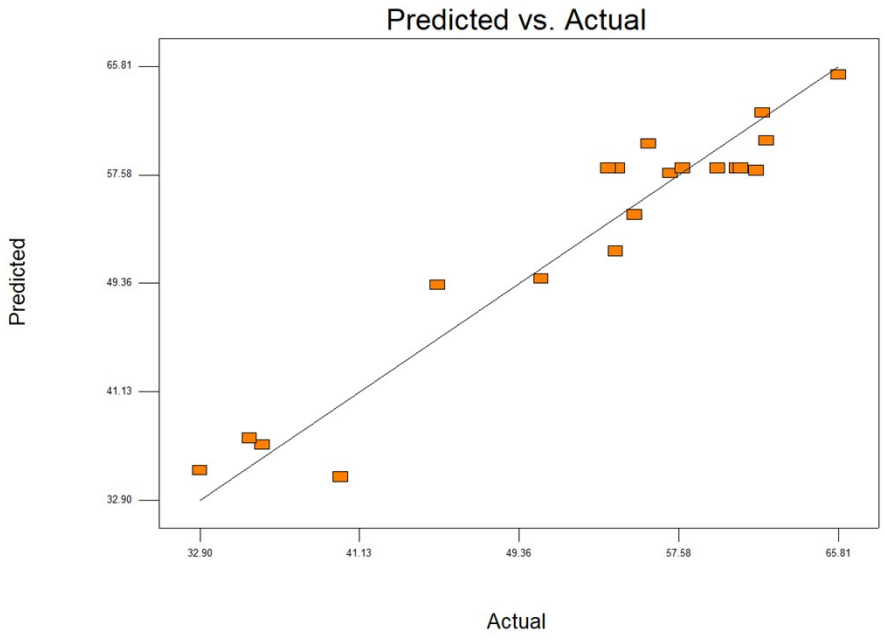

Figure 10: Predicted vs Actual DY%

Table S2: Sulphur content measured by ICP-MS for process optimisation

Sample	ID	Dilution ratio	IPCMS result (ppb)	Sulphur content (ppm)
Run 1	1.1	50	3530.47	176.52
Run 1	1.2	50	3532.64	176.63
Run 1	1.3	50	3501.56	175.08
Run 2	2.1	50	3744.28	187.21
Run 2	2.2	50	3368.46	168.42
Run 2	2.3	50	3772.19	188.61
Run 3	3.1	50	3434.65	171.73
Run 3	3.2	50	3386.16	169.31

Run 3	3.3	50	3161.92	158.10
Run 4	4.1	50	2854.26	142.71
Run 4	4.2	50	3506.92	175.35
Run 4	4.3	50	2910.96	145.55
Run 5	5.1	50	3123.63	156.18
Run 5	5.2	50	3371.74	168.59
Run 5	5.3	50	3062.01	153.10
Run 6	6.1	50	3293.65	164.68
Run 6	6.2	50	2862.07	143.10
Run 6	6.3	50	2800.01	140.00
Run 7	7.1	50	3528.02	176.40
Run 7	7.2	50	3542.79	177.14
Run 7	7.3	50	3320.51	166.03
Run 8	8.1	50	2603.06	130.15
Run 8	8.2	50	2745.14	137.26
Run 8	8.3	50	2735.02	136.75
Run 9	9.1	50	5201.15	260.06
Run 9	9.2	50	5263.83	263.19
Run 9	9.3	50	5398.01	269.90
Run 10	10.1	50	3633.48	181.67
Run 10	10.2	50	4228.38	211.42
Run 10	10.3	50	3841.69	192.08
Run 11	11.1	50	5474.47	273.72
Run 11	11.2	50	5206.21	260.31
Run 11	11.3	50	4575.42	228.77
Run 12	12.1	50	3758.52	187.93
Run 12	12.2	50	3326.34	166.32
Run 12	12.3	50	3712.68	185.63
Run 13	13.1	50	3591.38	179.57
Run 13	13.2	50	3591.38	179.57
Run 13	13.3	50	3591.38	179.57
Run 14	14.1	50	4198.75	209.94
Run 14	14.2	50	4441.67	222.08

Run 15	15.1	50	4320.21	216.01
Run 15	15.2	50	5130.76	256.54
Run 15	15.3	50	4566.87	228.34
Run 16	16.1	50	2815.57	140.78
Run 16	16.2	50	2876.34	143.82
Run 16	16.3	50	3389.71	169.49
Run 17	17.1	50	3103.09	155.15
Run 17	17.2	50	2907.95	145.40
Run 17	17.3	50	2995.61	149.78
Run 18	18.1	50	4619.40	230.97
Run 18	18.2	50	4596.58	229.83
Run 18	18.3	50	4245.59	212.28
Run 19	19.1	50	3391.45	169.57
Run 19	19.2	50	3634.00	181.70
Run 19	19.3	50	3106.89	155.34
Run 20	20.1	50	3162.57	158.13
Run 20	20.2	50	3044.11	152.21
Run 20	20.3	50	3114.98	155.75
Run 21	21.1	50	2892.69	144.63
Run 21	21.2	50	2980.21	149.01
Run 21	21.3	50	2727.42	136.37
Run 22	22.1	50	2415.95	120.80
Run 22	22.2	50	2296.60	114.83
Run 22	22.3	50	2534.52	126.73

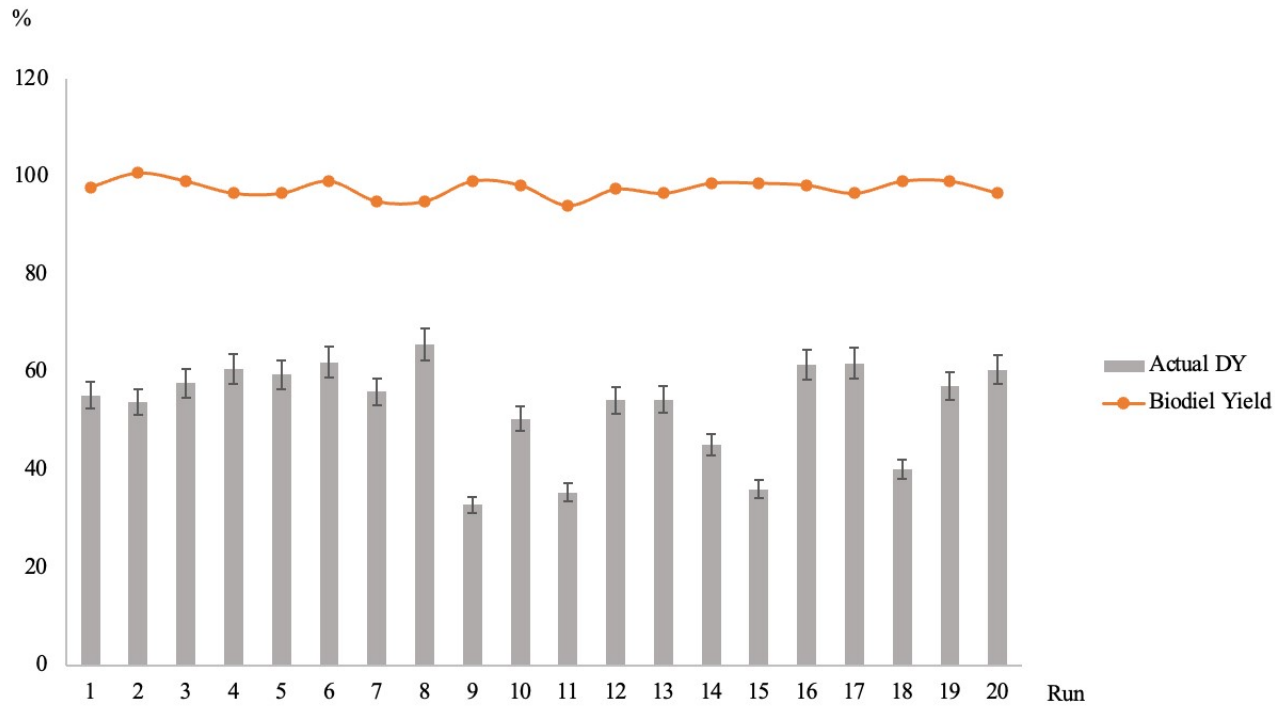

Figure 11: Diagram Actual DY and Biodiesel yield for 20 runs.

Table S3: Sequential model sum of square

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Mean	56349.73	1	56349.73			
Linear	846.14	3	282.05	4.5	0.018	
2FI	480.58	3	160.19	3.99	0.0324	
Quadratic	377.84	3	125.95	8.71	0.0039	Suggested
Cubic	91.72	4	2.93	2.6	0.1419	Aliased
Residual	52.86	6	8.81			
Total	58198.86	20	2909.94			

Table S4: Lack of fit

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Linear	957.15	11	87.01	9.49	0.0112	
2FI	476.57	8	59.57	6.5	0.0272	
Quadratic	931	5	19.75	2.15	0.2299	Suggested
Cubic	7.01	1	7.01	0.76	0.4219	Aliased
Pure Error	45.84	5	9.17			

Table S5: Model summary statistics.

Source	Std. Dev.	R-Squared	Adjusted R-Squared	Predicted R-Squared	PRESS	
Linear	7.92	0.4576	0.3559	0.0802	1700.79	
2FI	6.34	0.7175	0.5871	0.3432	1214.6	
Quadratic	3.8	0.9218	0.8515	0.5521	828.17	Suggested
Cubic	2.97	0.9714	0.9095	0.1862	1504.76	Aliased