Table S1. Material balance and energy stream data of the basic process

Material Streams											
		Isopropyl alcohol	Recycle	Pressurized Reactor Feed	3	Reactor Effluent	Partially Cooled Effluent	Flash Drum Feed	5	Liquid Separator Bottoms	Process water
Vapour Fraction		0.0000	0.0000	1.0000	1.0000	0.0000	0.5341	0.4140	1.0000	0.0000	0.0000
Temperature	C	25.00	61.24	234.0	350.0	350.0	45.00	20.00	20.00	20.00	27.00
Pressure	bar	2.300	1.200	2.160	1.910	1.910	1.770	1.630	1.630	1.630	1.630
Molar Flow	kgmole/h	51.96	3.151	55.11	86.46	0.0000	86.46	86.46	35.79	50.67	19.11
Mass Flow	tonne/h	2.401	0.1811	2.582	2.582	0.0000	2.582	2.582	0.3061	2.276	0.3443
Liquid Volume Flow	m^3/h	2.975	0.2290	3.204	4.014	0.0000	4.014	4.014	1.210	2.803	0.3450
Heat Flow	kW	-4432	-214.2	-3696	-3008	0.0000	-3873	-4014	-274.9	-3739	-1512
		Hydrogen	Light End Stream	Acetone	stream 12	13	Waste water	9	Combined Reactor Feed	2	
Vapour Fraction		1.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Temperature	C	34.34	26.88	61.50	81.56	61.24	89.94	21.52	26.76	26.82	
Pressure	bar	1.500	1.630	1.200	1.400	1.200	1.260	1.630	1.200	2.300	
Molar Flow	kgmole/h	34.93	19.97	30.20	40.44	3.162	37.28	70.64	55.11	55.11	
Mass Flow	tonne/h	0.2224	0.4280	1.716	0.9878	0.1817	0.8061	2.704	2.582	2.582	
Liquid Volume Flow	m^3/h	1.100	0.4550	2.169	1.090	0.2298	0.8599	3.258	3.204	3.204	
Heat Flow	kW	-222.4	-1564	-1812	-3142	-215.0	-2922	-5303	-4647	-4646	

Energy Streams										
		Q-101	Q-Rxn	Q-Cool	Q-102	Q-103	Q-104	Q-105	Q-106	Q-Pump
Heat Flow	kW	950.1	688.3	864.6	141.4	311.0	659.2	538.0	543.1	0.1341

Table S2. Material balance and energy stream data of the modified process

Material Streams													
		Isopropyl alcohol	Recycle	Preheated Reactor Feed	3	Liquid Residue	Cooled Reactor Effluent	5	Flash Drum Liquid Effluent	Process water	Hydrogen	Light End Stream	Acetone
Vapour Fraction		0.0000	0.0000	1.0000	1.0000	0.0000	0.4317	1.0000	0.0000	0.0000	1.0000	0.0000	1.0000
Temperature	C	25.00	61.24	234.0	350.0	350.0	20.00	20.00	20.00	27.00	34.35	26.88	61.50
Pressure	bar	2.300	1.200	2.160	1.910	1.910	1.630	1.630	1.630	1.630	1.500	1.630	1.200
Molar Flow	kgmole/h	51.96	3.202	55.16	86.51	0.0000	86.51	35.79	50.72	19.11	34.93	19.97	30.21
Mass Flow	tonne/h	2.401	0.1840	2.585	2.585	0.0000	2.585	0.3062	2.279	0.3443	0.2225	0.4280	1.717
Liquid Flow	m^3/h	2.975	0.2327	3.208	4.017	0.0000	4.017	1.210	2.807	0.3450	1.100	0.4550	2.169
Heat Flow	kW	-4432	-217.6	-3699	-3011	0.0000	-4017	-275.0	-3742	-1512	-222.5	-1564	-1813
		12	13	Waste water	9	Mechanical Work Input	2	Cooled_01	Heated_01	Precooled_01	Heated_ 02	Cooled_ 02	Heated_ 03
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000
Temperature	C	81.48	61.24	89.94	21.52	26.79	26.85	42.98	45.00	300.0	178.0	270.0	191.7
Pressure	bar	1.400	1.200	1.260	1.630	1.200	2.300	1.260	2.300	1.910	1.200	1.910	1.500
Molar Flow	kgmole/h	40.48	3.204	37.28	70.69	55.16	55.16	37.28	55.16	86.51	30.21	86.51	34.93
Mass Flow	tonne/h	0.9902	0.1841	0.8061	2.707	2.585	2.585	0.8061	2.585	2.585	1.717	2.585	0.2225
Liquid Flow	m^3/h	1.093	0.2328	0.8599	3.262	3.208	3.208	0.8599	3.208	4.017	2.169	4.017	1.100
Heat Flow	kW	-3145	-217.8	-2922	-5305	-4650	-4650	-2964	-4608	-3098	-1726	-3148	-172.2

Energy streams									
		Q-101	Q-Rxn	Q-102	Q-103	Q-104	Q-105	Q-106	Q-Pump
Heat Flow	kW	908.8	688.5	869.7	311.1	658.7	545.0	550.1	0.1343