

Additional file 1

Table S1: LF-NMR relaxometry data for pretreated materials, modified materials, and Avicel.

Substrate	DM %	mono-component T ₂ time, ms	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5		Peak 6		Peak 7	
			T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak	T ₂ time, ms	% water in peak
PS	5	1,350			10	2%	48	8%	353	17%	1550	74%				
	10	731			7	1%	41	17%	233	24%	965	57%				
	12	624			14	1%	44	11%	232	22%	767	66%				
	15	445	5.1	0.3%	-		33	8%	179	23%	533	69%				
	16.5	307	2.5	0.3%	-		30	10%	160	32%	411	58%				
	18	62	5.3	1.0%	19	10%	55	76%	166	13%						
	21	55	3.3	0.4%	14	6%	46	76%	106	17%						
	24	40	2.2	0.9%	15	17%	40	71%	52	11%						
	27	34	4.5	2.5%	12	8%	30	90%	76	7%						
	30	27	5.0	1.4%	11	9%	26	93%	18	7%						
PWS	5	1,043	8	1.3%	-		38	4%	-		198	18%	1,160	77%		
	7.5	1,082	4	1%	20	3.2%	-		74	8%	315	33%	1,512	54%		
	10	986	4	0.9%	13	2.9%	35	7%	60	8%	231	34%	1,052	57%		
	12	118	4	1.5%	20	12%	-		79	55%	217	31%	-			
	15	81	3	1.2%	13	7.2%	-		52	54%	131	37%	-			
	16.5	91	4	0.9%	16	12.7%	-		60	55%	171	31%	-			
	18	63	5	3.8%	12	7.0%	-		40	45%	89	44%				
	21	48	7	5.9%	-		-		28	47%	69	47%	-			
	24	38	4	3.1%	-		-		19	37%	49	60%	-			
	27	31	3	2.4%	-		-		14	31%	39	66%	-			
30	23	2	1.9%	-		-		11	28%	27	71%	-				

PWS milled	5	833	-	0.0 %	3	0.4 %	10	3%	32	7%	212	21 %	974	69 %		
	7.5	491	0.8	0.7 %	3	0.6 %	13	7%	39	10 %	180	29 %	677	53 %		
	10	264	0.5	0.9 %	8	4.2 %	-		26	15 %	136	37 %	405	43 %		
	12	147	0.4	0.5 %	3	1.2 %	-		17	16 %	69	30 %	206	52 %		
	15	107	0.4	1.0 %	3	0.7 %	-		15	16 %	50	34 %	159	49 %		
	16.5	85	0.2	1.0 %	1	0.9 %	-		11	12 %	36	35 %	122	51 %		
	18	76	0.1	0.9 %	1	0.7 %	-		10	10 %	33	38 %	110	50 %		
	21	50	0.7	0.9 %	6	0.9 %	-		6	5%	22	43 %	72	50 %		
	24	38	0.4	1.1 %	3		-		3	3%	17	44 %	52	52 %		
	27	30	0.3	1.3 %	2		-		2	2%	13	42 %	40	55 %		
	30	22	0.5	2.2 %	1		-		1	2%	10	35 %	27	63 %		
PWS de-lignified	5	382	1.07	0.5 %	7	0.7 %	30	3%	102	8%	321	73 %	865	16 %		
	7.5	206	0.35	0.2 %	5	0.9 %	26	5%	90	29 %	219	54 %	524	18 %		
	10	186	0.56	0.5 %	5	0.7 %	20	4%	66	21 %	167	57 %	446	18 %		
	12.0	145	0.88	0.2 %	2	0.4 %	11	2%	39	16 %	112	55 %	302	27 %		
	15	98	0.16	1.2 %	3	1.0 %	8	1%	25	14 %	69	55 %	188	28 %		
	16.5	95	-		3	1.1 %	15	7%	28	23 %	79	50 %	226	24 %		
	18	86	0.29	0.7 %	2	0.9 %	-		12	5%	42	47 %	112	40 %		
	21	61	0.49	1.5 %	3	1.1 %	-		16	15 %	45	51 %	124	31 %		
	24	41	0.24	0.5 %	3	1.8 %	-		-		20	36 %	52	62 %		
	27	27	0.59	1.4 %	-		-		-		11	19 %	30	80 %		
	30	20	0.63	1.3 %	1	1.8 %	-		-		9	31 %	24	67 %		
PWS xylanase	5	2384	-		6	1.4 %	25	5%	69	9%	171	25 %	424	13 %	3,262	47%
	7.5	805	-		6	1.7 %	28	7%	47	10 %	138	48 %	354	18 %	2,833	21%
	10	200	-		4	1.1 %	14	3%	42	13 %	116	49 %	260	26 %	1,754	8%
	12	122	0.19	1%	5	1.5 %	16	4%	41	17 %	109	60 %	262	16 %	-	
	15	94	0.61	1%	3	1.1 %	-		16	9%	56	46 %	145	44 %	-	
	16.5	80	0.56	1%	5	1.6 %	7	2%	27	20 %	74	62 %	208	14 %	-	
	18	67	0.76	1%	4	0.9 %	7	1%	18	12 %	52	59 %	123	27 %	-	
	21	60	0.36	1%	3	0.8 %	5	2%	20	20 %	54	62 %	142	15 %	-	-
	24	48	0.49	1%	5	2.2 %	-		18	24 %	44	56 %	141	17 %	-	-
	27	37	0.36	1%	2	0.9 %	3	2%	13	15 %	33	69 %	89	13 %	-	-

						%				%		%		%		
	30	31	0.20	1%	2	2.1%	6	6%	-		19	59%	51	36%	-	-
Avicel	5	3,918	6	1%	17	2%	-		95	13%	354	1%	4,060	83%		
	7.5	3,719	6	2%	22	2%	-		98	21%	343	2%	3,952	74%		
	10	3,539	4	1%	16	3%	38	3%	109	31%	282	4%	3,951	60%		
	12	3,395	6	3%	28	5%	-		104	35%	286	4%	3,898	53%		
	15	3,110	6	3%	27	7%	-		101	43%	282	6%	3,862	41%		
	16.5	2,752	3	1%	12	6%	42	7%	107	47%	316	7%	3,757	32%		
	18	1,971	10	4%	34	7%	-		100	49%	230	15%	3,576	23%		
	21	1,682	3	2%	13	7%	25	4%	76	51%	179	19%	3,536	19%		
	24	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR		
	27	83	5	2%	19	8%	-	15%	55	38%	117	44%	893	3%		
	30	63	6	6%	13	10%	-	22%	67	75%		1%		0%		

Legend: T₂ times of major peaks and relative amount of water in each peak for pretreated and modified materials measured at different % DM. Calculated from the areas of each peak relative to total under peak area, after NNLS analysis of the T₂ decay curves. T₂ times are reported as the T₂ time at maximum peak height. Data represents the average of triplicate samples. Peak number is arbitrary, and defined as the peak with the fastest T₂ relaxation time being peak 1, and increasing in peak number from there. Peak numbers between different substrates are not comparable, as some substrates and samples have more or fewer peaks. This data is represented in Figures 2 and 5 in the manuscript. NR stands for not recorded.