

Supplementary information

Supercritical Carbon Dioxide Extraction of Lignocellulosic Bio-Oils: The Potential of Fuel Upgrading and Chemical Recovery

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Table S1. Solubility data of bio-oil components at different temperature and pressure conditions.

Cyclohexanone							Ref.
P (bar) @ 160 °C	96	131	165	194	213		[139]
Solubility (g/kg)	83.0	118.8	149.4	195.0	258.2		
P (bar) @ 180 °C	89	135	175	209	215		
Solubility (g/kg)	118.8	162.4	191.5	276.0	293.4		
5-Hydroxymethylfurfural							Ref.
P (bar) @ 41 °C	97	116	133	148	166	187	[140]
Solubility (g/kg)	1.4	2.8	3.5	4.4	5.7	6.8	
P (bar) @ 51 °C	110	128	144	158	177	196	
Solubility (g/kg)	1.4	2.8	3.5	4.4	5.7	6.8	
P (bar) @ 61 °C	119	140	153	166	184		
Solubility (g/kg)	1.4	2.8	3.5	4.4	5.7		
P (bar) @ 70 °C	127	149	153	166	184		
Solubility (g/kg)	1.4	2.8	3.5	4.4	5.7		
Heptanoic Acid							Ref.
P (bar) @ 40 °C	100	115	150	175	200		[141]
Solubility (g/kg)	50.6	72.1	89.9	106.2	123.8		
P (bar) @ 50 °C	85	100	115	150	175	200	
Solubility (g/kg)	0.3	3.2	47.8	93.0	125.6	158.4	
P (bar) @ 60 °C	85	100	115	150	175	200	
Solubility (g/kg)	0.5	1.2	3.5	40.9	128.3	140.1	
Hexadecanoic Acid							Ref.
P (bar) @ 35 °C	99	127	157	186	206	230	[142]

Solubility (g/kg)	19.2	34.5	58.9											
Naphthalene													Ref.	
P (bar) @ 35 °C	86	97	105	131	167	197	220	239	252					[151]
Solubility (g/kg)	21.5	27.9	30.4	40.0	45.4	48.2	51.5	53.6	54					
P (bar) @ 55 °C	81	91	101	108	120	132	142	159	169	173	187	208		
Solubility (g/kg)	3.8	4.9	8.5	15.7	35.0	59.2	70.7	84.0	92.6	94.8	106.4	113.8		
P (bar) @ 55 °C	221	235	248	284										
Solubility (g/kg)	117.4	122.8	132.2	142.1										
P (bar) @ 60 °C	107	132	151	162	173	181	190	201	203	214	215	224		
Solubility (g/kg)	15.1	42.9	71.8	93.0	115.6	119.1	142.2	154.5	162.8	179.0	179.6	195.9		
P (bar) @ 60 °C	229	233	245	252	254	270	288							
Solubility (g/kg)	195.9	208.7	225.0	227.9	235.9	235.4	240.4							
P (bar) @ 65 °C	150	169	183	190	210	222	229							
Solubility (g/kg)	67.5	102.3	118.9	133.3	167.0	186.8	199.9							
P (bar) @ 121 °C	77	97	115	134	155	164							[152]	
Solubility (g/kg)	14.4	17.3	22.1	29.4	30.0	31.9								
P (bar) @ 162 °C	83	102	119	136	150	166								
Solubility (g/kg)	29.7	27.5	30.8	31.1	49.6	51.5								
Benzeneacetic Acid													Ref.	
P (bar) @ 35 °C	84	91	96	99	99	103	111	112	135	143	161	167	[153]	
Solubility (g/kg)	3.1	6.8	7.7	6.6	7.7	8.9	11.7	12.3	15.0	17.4	19.8	19.8		
P (bar) @ 35 °C	174	175	184											
Solubility (g/kg)	21.0	22.5	23.4											
P (bar) @ 45 °C	93	109	122	131	138	142	152	171	191					
Solubility (g/kg)	1.2	6.5	17.1	22.2	26.7	27.3	33.0	43.0	52.2					
Benzoic Acid													Ref.	
P (bar) @ 35 °C	101	113	120	151	160	240	280	282	364					[154]
Solubility (g/kg)	2.2	2.9	3.8	4.8	6.5	8.6	9.1	8.1	8.7					
P (bar) @ 45 °C	101	105	113	120	151	160	200	240	280	282	303	363		
Solubility (g/kg)	0.7	1.4	1.6	3.2	5.5	6.6	8.8	11.6	12.1	11.0	12.2	13.4		
P (bar) @ 55 °C	101	105	111	120	126	151	160	200	240	281	303	363		
Solubility (g/kg)	0.4	0.6	0.8	1.4	2.1	5.4	6.3	10.6	14.2	15.6	17.5	19.6		

P (bar) @ 70 °C	101	111	126	151	201	281	364							
Solubility (g/kg)	0.3	0.6	1.5	4.3	13.8	24.6	34.7							
P (bar) @ 45 °C	120	160	200	240	280									[155]
Solubility (g/kg)	3.2	6.5	8.8	11.6	12.1									
P (bar) @ 55 °C	120	160	200	240	280									
Solubility (g/kg)	1.4	6.3	10.6	14.2	20.1									
P (bar) @ 65 °C	120	160	200	240	280									
Solubility (g/kg)	0.9	4.8	11.3	19.1	26.8									
Phenol													Ref.	
P (bar) @ 60 °C	100	125	150	175	200	225	250	275	300	325	350			[156]
Solubility (g/kg)	2.4	11.4	28.6	49.1	74.0	83.1	90.8	109.5	119.9	134.6	151.9			
P (bar) @ 75 °C	100	125	150	175	200	225	250	275	300	325	350			
Solubility (g/kg)	3.9	7.4	15.6	34.2	57.9	74.5	82.2	111.9	124.0	139.6	158.4			
P (bar) @ 90 °C	100	125	150	175	200	225	250	275	300	325	350			
Solubility (g/kg)	4.4	6.9	15.9	24.3	41.4	58.0	79.2	104.4	130.1	152.3	175.5			
P (bar) @ 36 °C	79	81	87	97	106	111	119	124	133	146	147	156		[157]
Solubility (g/kg)	7.4	15.5	20.3	23.8	26.2	27.0	28.8	29.3	31.2	31.6	31.8	33.4		
P (bar) @ 36 °C	162	163	172	183	183	194	196	208	214	216	222	234	249	
Solubility (g/kg)	33.7	34.3	33.4	35.1	34.7	35.0	35.4	36.8	37.5	37.6	38.2	38.4	38.0	
P (bar) @ 60 °C	114	127	146	146	153	160	168	178	183	187	193	204		
Solubility (g/kg)	13.8	26.0	38.9	39.2	37.8	45.8	46.1	58.6	60.1	63.3	65.2	64.9		
P (bar) @ 60 °C	211	222	233	242										
Solubility (g/kg)	79.7	74.8	90.8	94.6										
P (bar) @ 100 °C	107	152	202	251	301									[158]
Solubility (g/kg)	11.9	23.0	52.2	97.7	164.5									
Catechol													Ref.	
P (bar) @ 60 °C	100	125	150	175	200	225	250	275	300	325	350			[156]
Solubility (g/kg)	0.3	0.8	2.7	4.1	5.0	5.7	6.5	6.8	7.4	7.5	7.6			
P (bar) @ 60 °C	100	125	150	175	200	225	250	275	300	325	350			
Solubility (g/kg)	0.4	0.9	1.4	2.6	3.8	4.8	5.9	6.7	7.7	8.7	9.6			
P (bar) @ 60 °C	100	125	150	175	200	225	250	275	300	325	350			

Solubility (g/kg)	0.5	0.7	1.1	2.3	3.7	4.9	6.0	7.2	9.1	10.1	11.4	
P (bar) @ 35 °C	122	162	203	243	284	324	365	405				[159]
Solubility (g/kg)	1.7	2.4	2.5	2.7	2.9	3.0	3.3	3.3				
P (bar) @ 45 °C	122	162	203	243	284	324	365	405				
Solubility (g/kg)	2.0	2.6	3.1	3.7	3.9	4.2	4.5	4.8				
P (bar) @ 55 °C	122	162	203	243	284	324	365	405				
Solubility (g/kg)	1.9	3.2	4.1	4.7	5.5	6.0	6.2	6.4				
P (bar) @ 65 °C	122	162	203	243	284	324	365	405				
Solubility (g/kg)	1.6	3.9	5.4	6.4	7.4	8.1	9.0	9.8				
Vanillin												Ref.
P (bar) @ 40 °C	87	117	149	174	187	198	205	227	235	259	273	[160]
Solubility (g/kg)	1.0	4.3	9.6	11.6	12.1	12.6	12.9	13.4	13.4	12.9	13.2	
P (bar) @ 60 °C	84	109	127	148	162	173	178	200	233	277		
Solubility (g/kg)	0.5	1.8	4.1	6.5	10.3	10.9	11.3	15.5	20.7	17.3		
P (bar) @ 80 °C	80	95	112	128	141	166	173	197	230	254	268	
Solubility (g/kg)	0.5	1.7	1.5	3.8	7.3	11.4	11.8	18.7	26.2	35.3	43.4	
P (bar) @ 35 °C	83	98	110	120	136	151	161	172	180	185	190	[153]
Solubility (g/kg)	1.3	3.9	5.1	5.3	6.5	7.5	8.0	8.3	8.9	9.0	9.6	
P (bar) @ 45 °C	98	113	120	131	145	155	163	170	178	185	195	
Solubility (g/kg)	1.5	4.2	5.1	6.8	8.1	8.6	8.8	9.7	10.2	10.9	12.1	
Solubility (g/kg)	10.3			52.3			96.3			147.1		[161]
T (°C)	83	105	71	94	119	136	88	103	123	95	107	122
P (bar)	216	249	414	391	385	389	664	592	528	807	711	658
Solubility (g/kg)		318.3										
T (°C)	74	79	94	102								
P (bar)	1341	1238	999	919								
Guaiacol												Ref.
P (bar) @ 50 °C	80	100	130	150	180							[162]
Solubility (g/kg)	2.4	14.9	107.6	156.0	260.5							
P (bar) @ 80 °C	80	100	130	160	200							
Solubility (g/kg)	3.2	5.9	16.6	50.2	144.5							
P (bar) @ 120 °C	80	100	130	160	200							
Solubility (g/kg)	10.7	13.3	19.2	32.0	62.5							
o-Cresol												Ref.

P (bar) @ 50 °C	102	142	201	250	268		[163]
Solubility (g/kg)	17.5	82.9	156.7	248.1	395.1 ₁		
P (bar) @ 200 °C	99	152	202	250	300		
Solubility (g/kg)	84.9	96.8	127.4	187.6	464.6 ₁		
P (bar) @ 100 °C	104	153	201	252	260	263	[158]
Solubility (g/kg)	11.0	27.1	74.7	203.0	270.6	392.5 ₁	
m-Cresol							Ref.
P (bar) @ 35 °C	80	100	120	160	200	240	[164]
Solubility (g/kg)	13.3	29.5	37.2	50.3	60.9	71.5	
P (bar) @ 45 °C	80	100	120	160	200	240	
Solubility (g/kg)	1.8	14.4	30.4	50.5	66.1	80.5	
P (bar) @ 55 °C	80	100	120	160	200	240	
Solubility (g/kg)	1.4	4.2	16.9	45.2	65.9	86.9	
P (bar) @ 100 °C	102	152	199	250	300		[158]
Solubility (g/kg)	7.6	18.2	45.9	92.0	169.1		
p-Cresol							Ref.
P (bar) @ 50 °C	100	150	200	250	301	348	[163]
Solubility (g/kg)	7.6	42.6	64.1	82.9	102.3	118.8	
P (bar) @ 200 °C	101	151	200	250	299	336	
Solubility (g/kg)	66.8	76.5	98.8	137.2	219.7	530.5 ₁	
P (bar) @ 80 °C	80	100	130	160	185	200	[162]
Solubility (g/kg)	2.6	4.1	10.0	24.7	42.6	53.8	
P (bar) @ 120 °C	80	100	130	160	200		
Solubility (g/kg)	8.5	10.4	14.7	22.9	41.5		
P (bar) @ 150 °C	80	100	130	160	200		
Solubility (g/kg)	20.1	21.7	27.1	35.6	49.6		
P (bar) @ 100 °C	103	154	202	251	302		[158]
Solubility (g/kg)	7.8	18.5	47.5	89.8	159.7		
¹ One phase was detected							