

Supporting Information

From Glucose-Based Carbohydrates to Phenol-rich Bio-oil Integrated with Syngas Production via Catalytic Pyrolysis over Activated Carbon Catalyst

Yayun Zhang^a, Hanwu Lei^{a,*}, Zixu Yang^a, Dengle Duan^a, Elmar Villota^a, Roger Ruan^b

^a. Department of Biological Systems Engineering, Washington State University, Richland, WA 99354-1671, USA

^b. Department of Bioproducts and Biosystems Engineering University of Minnesota, 1390 Eckles Ave., St. Paul, MN 55108, USA

Corresponding author. Tel.: +1 509 372 7628; fax: +1 509 372 7690. E-mail address:
hlei@wsu.edu (H. Lei).

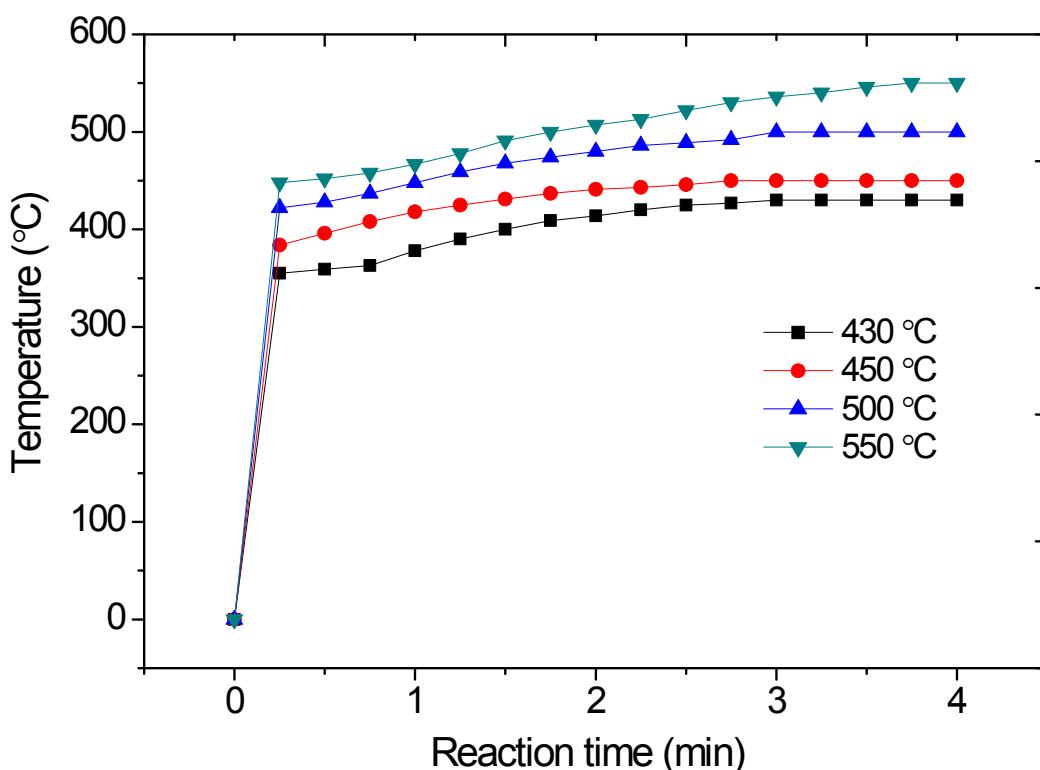


Figure S1. The temperatures change along with the initial 4 min of the reaction time.

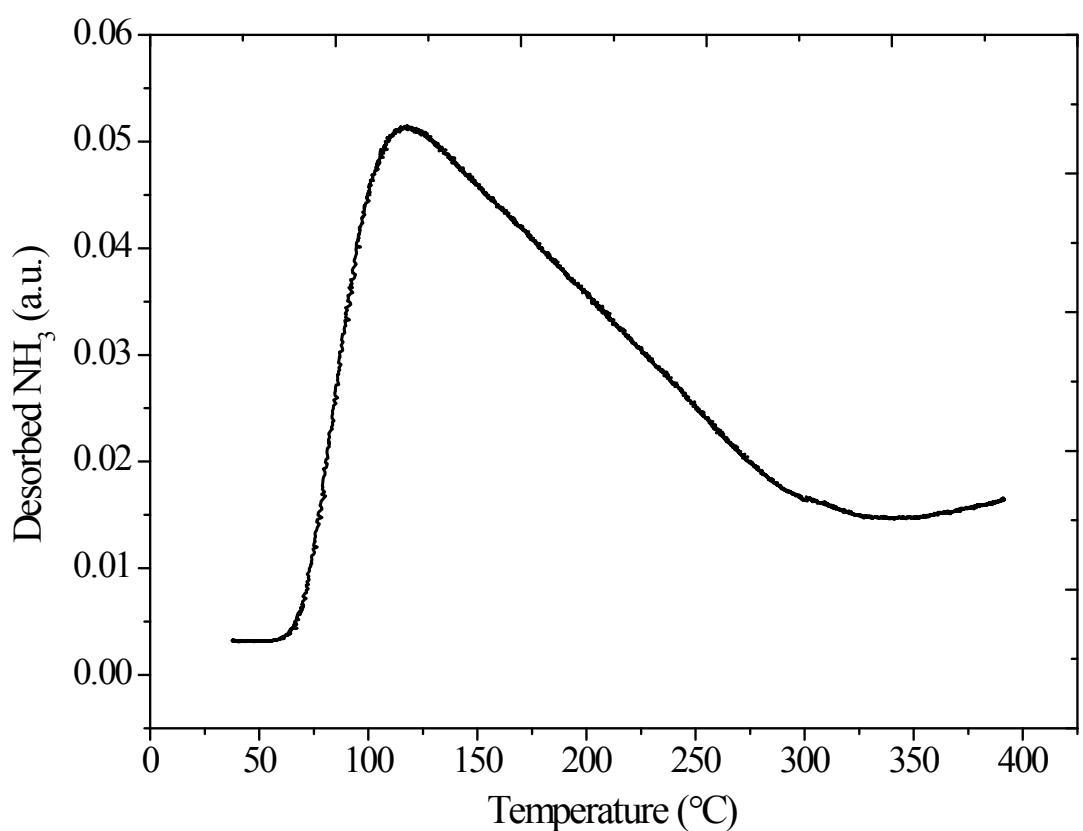


Figure S2 NH₃-TPD curve of the phosphoric acid activated ACC.

Table S1. The compositions of obtained oils in each run of catalytic pyrolysis of glucose.

RT (min)	Compound name	Category	Peak area (%)						
			R-1	R-2	R-3	R-4	R-5	R-6	R-7
4.6368	2(5H)-Furanone	Ketones			0.34	0.53		0.55	0.84
4.97	3-Furaldehyde	Aldehydes	1.02	-	0.47	0.97	-	0.81	1.74
5.35	Furfural	Furans	31.7 4	-	27.0 3	25.8 5	8.82	27.9 9	31.5 8
6.36	2-Hexanone, 3,4-dimethyl-	Ketones	-	-	1.87	-	-	-	-
6.45	2(3H)-Furanone, 5-methyl-	Furans						1.08	-
6.56	4-Hexen-2-one	Ketones				0.54	-	-	0.52
6.92-7.0	Cyclopent-4-ene-1,3-dione	Ketones			1.12	-	-	1.76	1.38
7.17	4-Cyclopentene-1,3-dione	Ketones	0.85	-	-	0.99	--	-	-
7.31	2,4-Dimethylfuran	Furans			2.79	-	-		1.87
7.45	Ethanone, 1-(2-furanyl)-	Ketones	3.89	-	4.51	5.83	-	3.73	-
8.01	2-Cyclopenten-1-one, 2-methyl-	Ketones					6.10	2.18	-
8.10-8.19	1,2-Cyclopentanedione	Ketones	-	-	3.30	0.95	-	1.44	1.12
8.89-8.77	2-Furancarboxaldehyde, 5-methyl-	Aldehydes	6.77	-	10.1 6	6.53	-	8.42	8.24
9.17	2-Cyclohexen-1-one	Ketones						1.25	1.30
9.319-9.4	Phenol	Phenols	48.1 7	10 0	15.3 4	30.5 7	77.5 2	23.5 1	32.9
10.34- 10.43	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	Ketones			4.89	-	-		-
10.52	Cyclooctene	Hydrocarbons				2.93	--	3.5	3.43
10.93	Phenol, 2-methyl-	Phenols			0.74	1.34	-	0.84	1.28
11.36- 11.43	Oxetane, 2-propyl-	Ketones			2.12	0.89	-	0.95	0.72
11.71- 11.65	Levoglucosenone	Anhydrosugar			15.3 4	20.2 5	-	18.4 5	11.2 0
12.167	Phenol, 3-methyl-	Phenols	5.87	-	-	-	7.51	-	-
13.58	1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	Anhydrosugar			5.17	1.52	-	1.51	-
14.47	1H-Inden-1-one, 2,3-dihydro-	Ketones			1.5	-	-	-	-
15.46	2-Acetylcylohexanone	Ketones						0.70	0.66
16.07- 16.18	Phenol, 2-methoxy-4-propyl-	Guaiacols		-	-	-	-	0.66	0.75
17.04	Ethanone, 1-(4,5-diethyl-2-methyl-1-cyclopenten-1-yl)-	Ketones						0.67	0.46
17.34	1,2-Dimethoxy-4-n-propylbenzene	Guaiacols				0.34	-	-	
19.77	Bicyclo[3.2.2]nona-2,6-dien-5-ol-4-	Phenols			0.32	-	-	-	-

	one							
--	-----	--	--	--	--	--	--	--

Table S1. The compositions of obtained oils in each run of catalytic pyrolysis of glucose (continue).

RT (min)	Compound name	Category	Peak area (%)							
			R-8	R-9	R-10	R-11	R-12	R-13	R-14	
4.6368	2(5H)-Furanone	Furans	0.71	0.67	0.43			0.51	0.43	
4.97	3-Furaldehyde	Aldehydes	1.09	0.87	0.36	0.73		0.97	0.65	
5.35	Furfural	Furans	23.6 8	25.4 7	25.7 8	27.9 3	19.5 4	24.0 1	28.6	
6.36	2-Hexanone, 3,4-dimethyl-	Ketones	-	-	2.28	1.49				
6.56	4-Hexen-2-one	Ketones							1.84	
6.45	2(3H)-Furanone, 5-methyl-	Ketones	0.85	1.38					1.13	
6.92-7.0	Cyclopent-4-ene-1,3-dione	Ketones	0.69	1.58	1.07	0.96	-	0.92	1.82	
7.31	2-Cyclopenten-1-one, 2-methyl-	Ketones	1.44	1.86	2.36	2.73	-	1.22	2.48	
7.45	Ethanone, 1-(2-furanyl)-	Ketones	2.61	3.02	4.07	2.98	2.62	2.91	4.79	
7.87	2(5H)-Furanone	Ketones				0.65				
8.10-8.19	1,2-Cyclopentanedione	Ketones	0.94	1.77	3.54	2.05	-	0.91	2.64	
8.89-8.77	2-Furancarboxaldehyde, 5-methyl-	Aldehydes	6.97	7.75	9.71	8.38	-	8.39	9.98	
9.17	2-Cyclohexen-1-one	Ketones		1.0	1.73	3.96		0.99		
9.319-9.4	Phenol	Phenols	28.5 1	25.7 4	4.75	12.9 5	74.7	19.5 1	19.7 9	
10.34- 10.48	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	Ketones			4.99	4.13	-	3.31	4.32	
10.52	Cyclooctene	Hydrocarbons	3.07	3.51			--	-		
10.93	Phenol,2-methyl-	Phenols	0.96	0.86	1.15	0.76	0.8	0.94	0.4	
11.36- 11.43	Oxetane, 2-propyl-	Ketones	0.69	1.0	1.61	1.69	-	0.86	1.92	
11.71- 11.65	Levoglucosenone	Anhydrosugar	25.7 1	20.3 2	18.7 6	17.0 6	-	29.9 7	10.2 3	
12.167	Maltol	Ketones	-	-	1.89	-	-	-	1.37	
12.66	4H-Pyran-4-one, 5-hydroxy-2-methyl-	Ketones			0.41				0.86	
12.84	3,6-Dimethyl-1-heptyn-3-ol	Ketones	-			0.64	-	-		
13.95- 13.86	1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	Anhydrosugar	1.32	1.45	8.70	5.62	-	2.66	3.78	
14.47	1H-Inden-1-one, 2,3-dihydro-	Ketones			1.55	2.58	-	0.39	-	
14.61	Catechol	Phenols							1.27	
14.86	2-(3'-Oxo-butyl)-cyclopentanone	Ketones			1.48					
15.04	Benzoinic acid	Acids					2.34			

15.59	2(5H)-Furanone, 5-(1-methylethyl)-	Ketones	0.35	0.5					
16.07-16.18	3,5-Octadiene, 4,5-diethyl-, (E,Z)-	Ketones		0.74	0.34	-	-		-
16.83	2(5H)-Oxepinone, 6,7-dihydro-	Ketones			0.87				
17.04	Ethanone, 1-(4,5-diethyl-2-methyl-1-cyclopenten-1-yl)-	Ketones	0.39	0.53	0.39			0.39	-
17.34	5,7-Dodecadiene, (Z,Z)-	Ketones			0.5		-		

Table S1. The compositions of obtained oils in each run of catalytic pyrolysis of glucose (continue).

RT (min)	Compound name	Category	Peak area (%)							
			R-15	R-16	R-17	R-18	R-19	R-20	R-21	
3.2	2-Pentene, 4-methyl-, (E)-	Hydrocarbons	2.11	0.90						
4.57	2(5H)-Furanone	Ketones			0.77	0.71	0.52	0.66	0.79	
4.97	3-Furaldehyde	Aldehydes	0.56	0.78						
5.35	Furfural	Furans	28.8 3	23.1 2	31.8 0	31.5 5	30.2 9	32.3 0	31.2 8	
6.36	2-Hexanone, 3,4-dimethyl-	Ketones	2.58							
6.40	4-Hexen-2-one	Ketones		4.95						
6.45	2(3H)-Furanone, 5-methyl-	Ketones			5.39	5.63	4.68	5.03	4.42	
6.92-7.0	Cyclopent-4-ene-1,3-dione	Ketones	0.97	0.73	0.67	0.84	0.88	0.86	0.75	
7.17	2(3H)-Furanone, dihydro-4-hydroxy-	Ketones		-	-			-	0.62	
7.31	2-Cyclopenten-1-one, 2-methyl-	Ketones				0.55	0.6	0.64	0.8	
7.45	Ethanone, 1-(2-furanyl)-	Ketones	4.4	5.20	5.05	4.38	3.97	4.02	3.68	
8.01	2-Cyclopenten-1-one, 2-methyl-	Ketones	3.6	3.58					-	
8.06	2-Pentenal, 2-methyl-	Aldehydes		2.01						
8.10-8.19	1,2-Cyclopentanedione	Ketones	4.18		1.06	1.12	1.27	1.24	1.51	
8.31	2(5H)-Furanone, 5-methyl-	Ketones			1.63	1.8	1.77	1.61	1.53	
8.49	2,3-Dimethyl-4-hydroxy-2-butenoic lactone	Ketones		2.29						
8.89-8.77	2-Furancarboxaldehyde, 5-methyl-	Aldehydes	10.1 7	11.6 9	7.89	8.46	8.06	8.11	7.79	
9.38	3-Methyl-3-cyclohexen-1-one	Ketones		1.69						
9.17	2-Cyclohexen-1-one	Ketones	0.96							
9.319-9.4	Phenol	Phenols	15.7 2	8.99						
9.81	3,4-Hexanedione	Ketones			2.38	2.58	2.67	2.69	2.76	
10.34-10.48	2-Cyclopenten-1-one,2-hydroxy-3-methyl-	Ketones	4.96	5.53	6.18	6.38	6.34	5.93	5.83	

10.93	Phenol,2-methyl-	Phenols	1.15	0.68			0.69	0.75	0.75
11.36- 11.43	Oxetane, 2-propyl-	Ketones	2.56	1.54	4.53	5.02	5.04	4.75	4.56
11.71- 11.65	Levoglucosenone	Anhydrosu ger	7.0	13.4 2	4.92	4.62	4.13	4.67	4.46
12.35	Maltol	Ketones	1.04	0.83	1.66	1.19	1.04	0.97	1.03
12.59	4H-Pyran-4-one, 5-hydroxy-2- methyl-	Ketones		0.41					
12.66	2-Propenoic acid, 2-methyl-, oxiranylmethyl ester	Acids			1.02	0.88	0.66	0.64	0.72
12.84	Phenol, 3,4-dimethyl-	Phenols	0.87						
13.58	4H-Pyran-4-one, 3,5-dihydroxy-2- methyl-	Ketones	-	0.93		-	-	-	-
13.68	1,4:3,6-Dianhydro-.alpha.-d- glucopyranose	Anhydrosu ger	5.75	5.54	14.8 6	14.1 8	15.9 9	14.8	16.2
14.44	1H-Inden-1-one, 2,3-dihydro-	Ketones	1.35	0.94					
14.47	5-Hydroxymethylfurfural	Aldehydes			5.56	5.38	6.06	4.44	4.81
14.86	2(5H)-Furanone, 5-(1- methylethyl)-	Ketones	0.56	1.04					
15.56	3,5-Octadiene, 4,5-diethyl-, (E,Z)-	Ketones		0.5	0.75	0.55	0.58	0.57	0.81
16.44	Ethanone, 1-(4,5-diethyl-2-methyl- 1-cyclopenten-1-yl)-	Ketones		0.98	0.49	0.43	0.54	0.56	0.6
16.83	2(5H)-Oxepinone, 6,7-dihydro-	Ketones		0.80	2.14	2.01	2.33	2.23	2.33
17.34	5,7-Dodecadiene, (E,Z)-	Ketones		0.26	0.44	0.39	0.43	0.45	0.43

Table S2. The main compositions of obtained oils with fresh, spent, regenerated, and HZSM-5 catalysts, respectively.

RT (min)	Compound name	Category	Peak area (%)
----------	---------------	----------	---------------

			Fresh	Spent	Regenerated	HZSM-5
4.08	Cyclopentanone	Ketones	-	-	5.29	-
4.55	Carbonocyanidic acid, ethyl ester	Other				1.63
4.6368	2(5H)-Furanone	Ketones		1.36	-	-
4.97	3-Furaldehyde	Aldehydes	-	0.84	-	-
5.35	Furfural	Furans	8.82	8.82	-	14.45
5.61	3-Cyclopentene-1-acetaldehyde, 2-oxo-	Ketones			7.46	
6.36	2-Hexanone, 3,4-dimethyl-	Ketones	-	7.49	-	-
6.45	2(3H)-Furanone, 5-methyl-	Furans		-	-	8.52
6.56	4-Hexen-2-one	Ketones	-	-	-	-
6.92-7.0	Cyclopent-4-ene-1,3-dione	Ketones	-	0.58	-	0.66
7.17	4-Cyclopentene-1,3-dione	Ketones	--	-	-	1.85
7.31	2,4-Dimethylfuran	Furans	-	1.55		-
7.45	Ethanone, 1-(2-furanyl)-	Ketones	-	4.9	-	3.63
8.01	2-Cyclopenten-1-one, 2-methyl-	Ketones	6.10	6.10	2.11	-
8.10-8.19	1,2-Cyclopentanedione	Ketones	-	2.09	-	1.22
8.89-8.77	2-Furancarboxaldehyde, 5-methyl-	Aldehydes	-	7.43	-	6.23
9.17	2-Cyclohexen-1-one	Ketones			-	2.35
9.319-9.4	Phenol	Phenols	77.57	3.45	62.3	-
10.34-10.43	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	Ketones	-		-	-
10.52	Cyclooctene	Hydrocarbons	--	8.75	-	3.43
10.93	Phenol, 2-methyl-	Phenols	-	-	3.28	1.28
11.36-11.43	Oxetane, 2-propyl-	Ketones	-	2.47	-	0.72
11.71-11.65	Levoglucosenone	Anhydrosugar	-	12.89	-	14.78
12.167	Phenol, 3-methyl-	Phenols	7.51	7.51	11.25	-
13.58	1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	Anhydrosugar	-	16.96	-	17.94
14.47	1H-Inden-1-one, 2,3-dihydro-	Ketones	-	1.15	-	-
14.97	Phenol, 3,4-dimethyl-	Phenols			8.58	
15.46	2-Acetylcylohexanone	Ketones		2.02	-	0.66
16.07-16.18	Phenol, 2-methoxy-4-propyl-	Guaiacols	-	-	-	0.75
17.04	Ethanone, 1-(4,5-diethyl-2-methyl-1-cyclopenten-1-yl)-	Ketones		0.52	-	0.46
17.34	1,2-Dimethoxy-4-n-propylbenzene	Guaiacols	-	1.92-	-	
19.77	Bicyclo[3.2.2]nona-2,6-dien-5-ol-4-one	Phenols	-	-	-	-