

Supplementary Information for the manuscript:

The effect of temperature, heating rate, and ZSM-5 catalyst on the product selectivity of the fast pyrolysis of Spent Coffee Grounds

Ari Fischer*, Shoucheng Du*, Julia A. Valla and George M. Bolas†

Chemical & Biomolecular Engineering, University of Connecticut, Storrs, Connecticut, 06269

Corresponding author:

George M. Bolas

Department of Chemical & Biomolecular Engineering, University of Connecticut

191 Auditorium Road Unit 3222

Storrs, Connecticut 06269-3222 USA

Tel: 860 486 4602

Email: george.bollas@uconn.edu

Abstract

Supplementary material for the manuscript “The effect of temperature, heating rate, and ZSM-5 catalyst on the product selectivity of the fast pyrolysis of Spent Coffee Grounds” is given. GC-MS chromatograph area percentage reports for liquid analysis of the fixed-bed and pyroprobe bio-oil are provided in Tables S1 and S2.

Table S1: Liquid selectivity of the liquid product from pyrolysis in the fixed-bed by GC-MS peak area percentage.

Compound	763	763	813	813	863	863
	Thermal	Catalytic	Thermal	Catalytic	Thermal	Catalytic
2-5-Dimethylfuran	0.7	0.4	0.0	0.0	0.8	0.3
Toluene	0.4	1.1	0.0	4.8	0.4	6.1
2-Cyclopenten-1-one	0.3	0.0	0.0	0.0	0.5	0.0
2-Furanmethanol	3.2	0.0	6.0	0.0	4.3	0.0
p-Xylene	0.0	1.8	0.0	3.1	0.0	4.7
2-Hydroxy-2-cyclopenten-1-one	2.0	1.5	0.0	0.0	0.0	0.0
Phenol	2.5	3.0	3.9	4.7	4.3	3.0
3-Methyl-1,2-cyclopentendione	1.8	0.0	0.0	0.0	2.1	1.0
2-Cyclopenten-1-one	0.0	1.5	0.0	1.1	0.0	0.0
Indene	0.0	0.0	0.0	1.8	0.0	0.9
2-Methylphenol	0.0	0.0	0.0	1.1	1.0	1.0
4-Methylphenol	2.0	2.9	3.2	3.8	3.2	2.3
1-Undecene	0.0	0.0	0.0	0.0	1.0	2.4
2,4-Dimethylphenol	0.0	1.0	1.1	1.5	1.2	0.0
Naphthalene	0.0	1.5	0.0	2.2	0.0	1.9
1-Dodecene	2.9	0.0	0.0	0.0	2.5	1.3
1,2-Benzenediol	1.8	3.7	4.0	2.9	5.2	3.5
Hydroquinone	2.0	1.1	2.1	1.7	1.3	2.8
1-Methylnaphthalene	0.0	3.6	0.0	3.1	0.0	1.2
1-Tridecene	0.0	0.0	1.0	0.0	3.2	0.0
Tridecane	0.0	0.0	0.6	0.0	1.0	1.8
(2-4)-Methyl-1H-indole	0.5	0.7	0.6	1.8	0.6	1.3
1-Tetradecene	1.5	0.5	1.6	0.9	4.1	1.2
Tetradecane	0.7	0.0	1.1	1.6	1.2	1.1
1-Pentadecene	0.5	0.0	0.0	0.0	1.6	0.9
Pentadecane	3.2	2.4	4.3	4.0	5.1	3.1
1-Hexadecene	0.0	0.0	0.6	0.0	0.9	0.0
Hexadecane	0.0	0.0	0.5	0.0	0.5	0.0
Heptadecane	1.3	1.1	1.9	1.9	2.0	1.1
Caffeine	7.7	7.1	8.3	5.4	8.4	3.8
Hexadecanenitrile	1.8	3.1	3.2	4.8	3.1	3.0
Hexadecanoic acid	40.7	39.6	36.9	28.4	23.1	26.7
Heptadecanenitrile	0.0	0.0	0.0	1.8	0.0	0.0
9,12-Octadecadienoic acid (Z,Z)-	14.2	13.5	9.8	10.4	5.9	8.7
Octadecanoic acid	5.7	6.5	6.6	4.3	3.7	2.0
Hexadecanamide	1.3	1.1	2.0	2.0	1.6	1.8

Table S2: Liquid selectivity of the liquid product from pyrolysis in the pyroprobe by GC-MS peak area percentage.

	763 Thermal	763 Catalytic	813 Thermal	813 Catalytic	863 Thermal	863 Catalytic
Benzene	0.0	6.8	0.0	6.6	0.0	6.4
Toluene	4.5	17.7	4.5	17.1	4.7	17.1
Pyridine, 2-methyl-	0.6	0.3	0.7	0.2	0.7	0.3
2-Furanmethanol	8.4	0.0	8.8	0.0	8.3	0.0
p-Xylene	0.0	15.0	0.0	16.0	0.0	15.1
Pyridine, 3-methyl-	3.3	0.0	2.8	0.0	3.4	0.0
Styrene	2.6	2.1	3.3	2.1	2.9	2.3
2-Cyclopenten-1-one, 2-methyl-	0.0	0.8	0.0	0.9	0.0	0.9
4,4-Dimethyl-2-cyclopenten-1-one	0.0	0.3	0.0	0.4	0.0	0.4
1,2-Cyclopentanedione	0.0	2.0	0.0	1.8	0.0	0.8
Pyridine, 2,4-dimethyl-	0.9	0.0	0.8	0.0	0.6	0.0
Benzene, 1-ethyl-2-methyl-	0.0	1.9	0.0	2.0	0.0	1.9
2-Furancarboxaldehyde, 5-methyl-	0.0	1.0	0.0	1.0	0.0	1.0
Phenol	7.8	5.4	8.3	5.6	7.4	6.1
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	1.3	0.8	1.4	0.8	1.6	1.1
Phenol, 2-methyl-	0.0	0.3	0.0	0.2	0.0	0.4
Phenol, 3-methyl-	1.8	1.0	2.2	0.6	2.0	1.4
Phenol, 4-methyl-	5.9	3.5	6.7	3.7	6.4	3.8
Mequinol	4.1	0.0	4.0	0.0	3.5	0.0
2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	1.1	1.0	1.2	0.8	1.3	0.7
1-Phenyl-1-butene	0.0	0.4	0.0	0.4	0.0	0.4
Benzyl nitrile	1.6	0.6	1.5	0.5	1.6	0.5
Benzene, 1-butynyl-	0.0	1.9	0.0	1.9	0.0	1.8
Triquinacene	1.4	0.0	1.5	0.0	1.6	0.0
Phenol, 3,5-dimethyl-	1.3	0.9	0.9	0.9	0.6	0.9
Naphthalene	0.0	5.2	0.0	5.0	0.0	5.4
Cyclododecane	1.2	0.7	1.2	0.6	1.4	0.6
Phenol, 2-methoxy-4-methyl-	1.1	0.8	1.1	0.7	1.3	0.8
1H-Indene, 1,1-dimethyl-	0.0	0.7	0.0	0.7	0.0	0.0
Naphthalene, 1-methyl-	0.0	6.5	0.0	6.4	0.0	6.2
1-Tridecene	0.8	0.0	0.7	0.0	0.8	0.0
Indole	1.7	0.0	1.9	0.0	1.8	0.0
Tridecane	0.5	0.5	0.6	0.6	0.4	1.4
2-Methoxy-4-vinylphenol	4.0	2.3	3.6	2.1	3.6	2.0
1H-Indole, 3-methyl-	1.2	0.9	1.4	0.8	1.4	1.1
2-Tetradecene, (E)-	1.3	0.8	1.5	0.8	1.2	0.9
Tetradecane	1.5	0.0	1.5	0.0	1.1	0.0
Naphthalene, 2,7-dimethyl-	0.0	2.5	0.0	2.3	0.0	2.5
Phenol, 2-methoxy-4-(1-propenyl)-	0.9	0.4	0.9	0.6	0.9	0.5
1-Pentadecene	1.1	0.3	1.2	0.4	1.1	0.8
Pentadecane	4.5	0.8	4.2	0.9	3.8	2.8

3-Hexadecene, (Z)-	0.0	2.7	0.0	3.1	0.0	0.3
Cyclododecane	0.6	0.0	0.6	0.0	0.5	0.0
5-Hexadecyne	0.0	0.3	0.0	0.3	0.0	0.3
Z,Z-10,12-Hexadecadienal	2.5	0.0	2.6	0.0	2.2	0.0
8-Heptadecene	2.9	0.3	3.1	0.3	2.4	0.3
Heptadecane	1.5	0.9	1.5	0.9	1.3	0.8
1-Pentadecene	0.4	0.3	0.4	0.3	0.4	0.3
Z,Z-10,12-Hexadecadienal	0.7	0.0	0.6	0.0	0.5	0.0
Caffeine	0.6	0.0	0.0	0.0	0.0	0.0
Hexadecanenitrile	1.2	1.1	1.4	1.1	1.2	1.1
Hexadecanoic acid, methyl ester	0.5	0.2	0.6	0.2	0.5	0.2
n-Hexadecanoic acid	19.1	7.6	17.9	8.3	16.0	8.3
9,12-Octadecadienoic acid (Z,Z)-	2.9	0.3	1.9	0.1	5.0	0.8
Octadecanoic acid	0.5	0.2	0.6	0.3	4.6	0.6
