Enhancing the Efficacy of the Subcritical Water-Based Alkali Lignin Depolymerization by Optimizing the Reaction Conditions and Using Heterogeneous Catalysts

Balawanthrao Jadhav[1*], Ranen Roy[1], Md Sajjadur Rahman[1], Tanvir A. Amit[1], Shiksha Subedi[1], Matthew Hummel[2], ZhengRong Gu[2], and Douglas E. Raynie[1]*

[1]Department of Chemistry and Biochemistry, South Dakota State University, Brookings, SD-57007, USA

[2]Department of Agricultural and Biosystem Engineering, South Dakota State University, Brookings, SD-57007, USA

*Corresponding Author: douglas.raynie@sdstate.edu

Table S1. Properties of water and subcritical water [1, 2]

Properties	Normal water	Subcritical water
Temperature (K)	298	523
Pressure (bar)	1	50
Density (g/cm^3)	1	0.80
Dielectric constant	78.5	27.1
p^{K}_{w}	14.0	11.2
Heat capacity (kJ/Kg K)	4.22	4.86
Dynamic viscosity (mPa s)	0.89	0.11
Heat conductivity (Mw/m K)	608	620

Table S2. Phenolic monomers and retention time.

Peak No	Retention time (min)	Phenolic monomer	Molecular weight	Moiety
1	3.121	Phenol	94	H
2	3.899	Guaiacol	124	G
3	5.024	Ethyl guaiacol	152	G
4	5.467	Vinyl guaiacol	150	G
5	5.831	Propyl guaiacol	166	G
6	6.095	Vanillin	152	G
7	6.365	Isoeugenol	164	G
8	6.627	Acetovanillone	166	G
9	6.895	Guaiacylacetone	180	G
10	7.226	Butyrovanillone	194	G
11	7.607	Homovanillic acid	182	G
12	8.155	Coniferylaldehyde	178	G

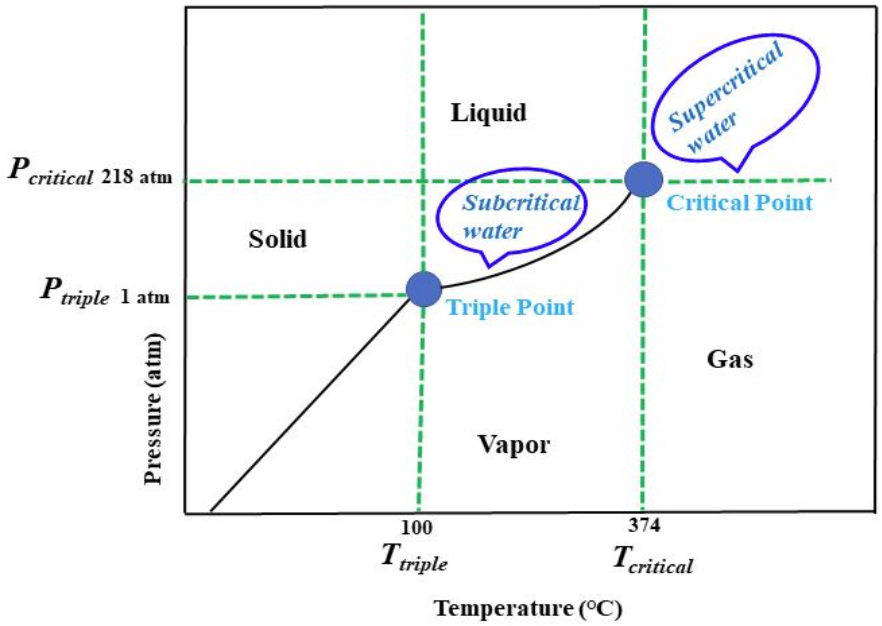

Figure S1. Phase diagram of water representing sub and supercritical region.

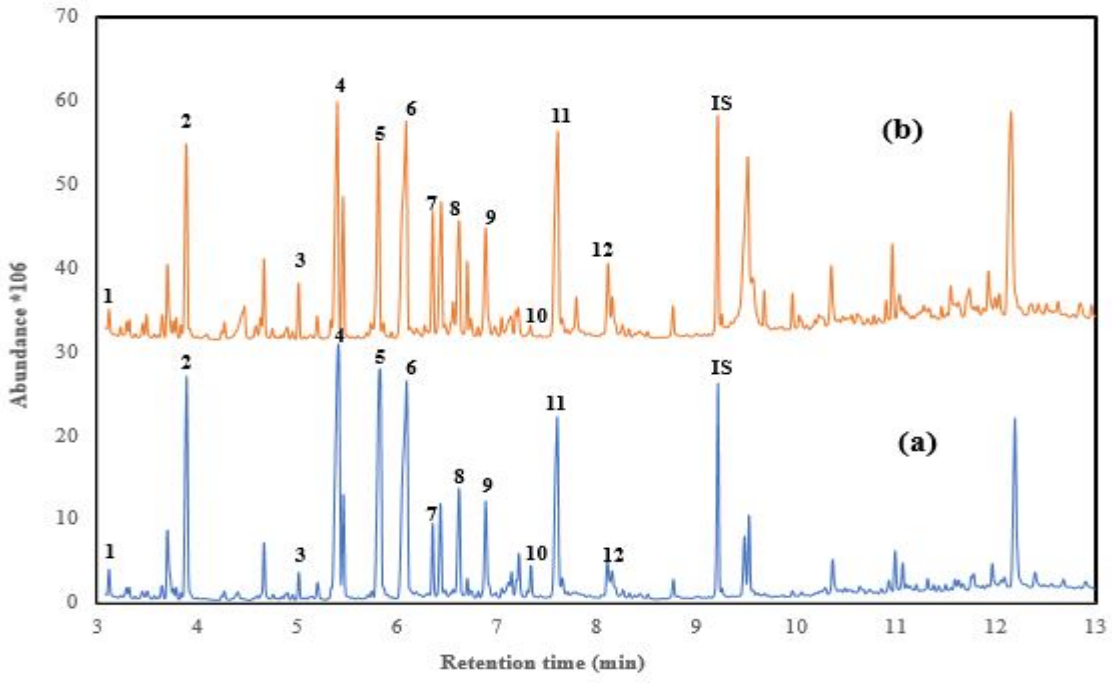

Figure S2. GCMS chromatogram of phenolic monomers from the alklali lignin in the presence of (a) 5 % V/Zeolite (b) 1.7% V/ZrO_2 (Sulfate)

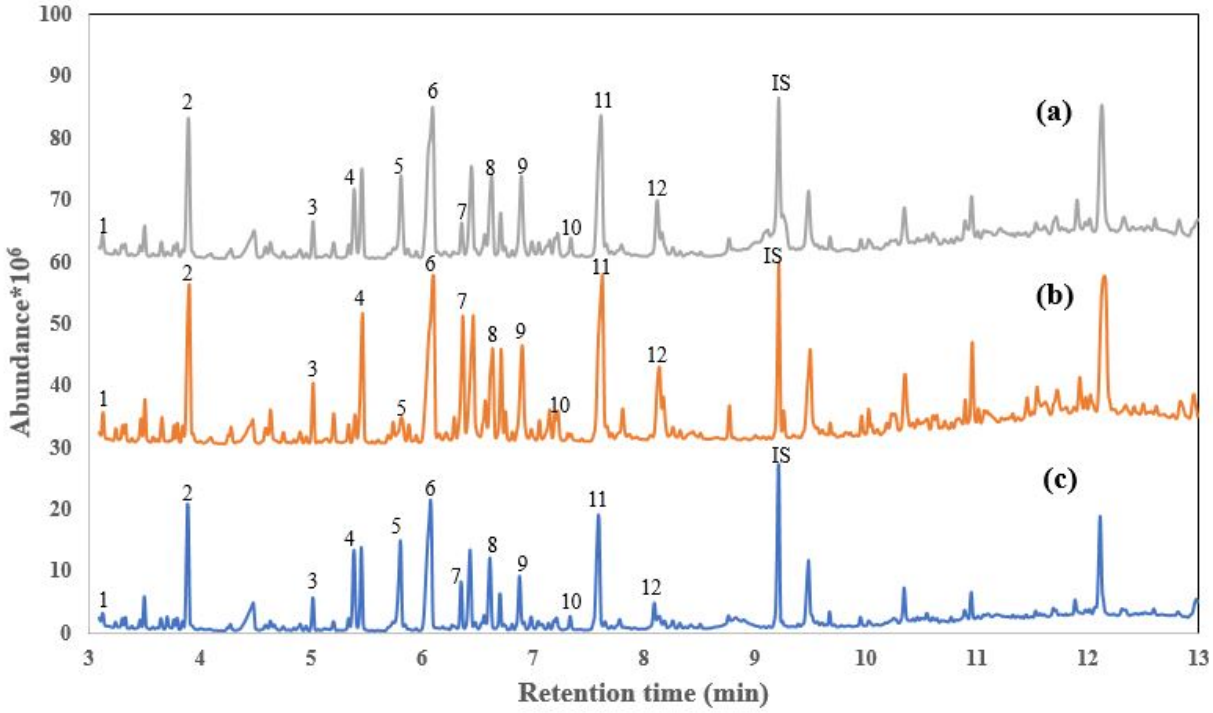

Figure S3. GCMS chromatogram of phenolic monomers from the alklali lignin in the presence of (a) 1.7% V/ZrO_2(Neutral) (b) Ni-Graphene (c) Ni-Zinc catalysts.

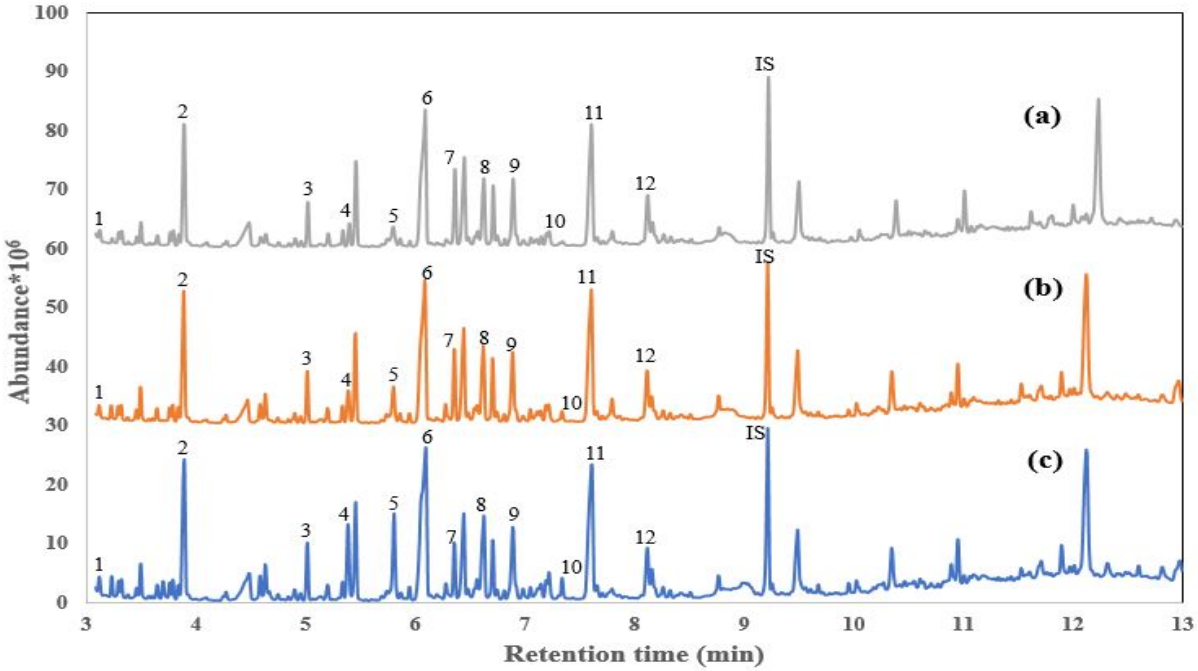

Figure S4. GCMS chromatogram of phenolic monomers from the alklali lignin in the presence of (a) 5 % V/Ni-Graphene (b) 1.7 % V/Zeolite (c) No catalysts.

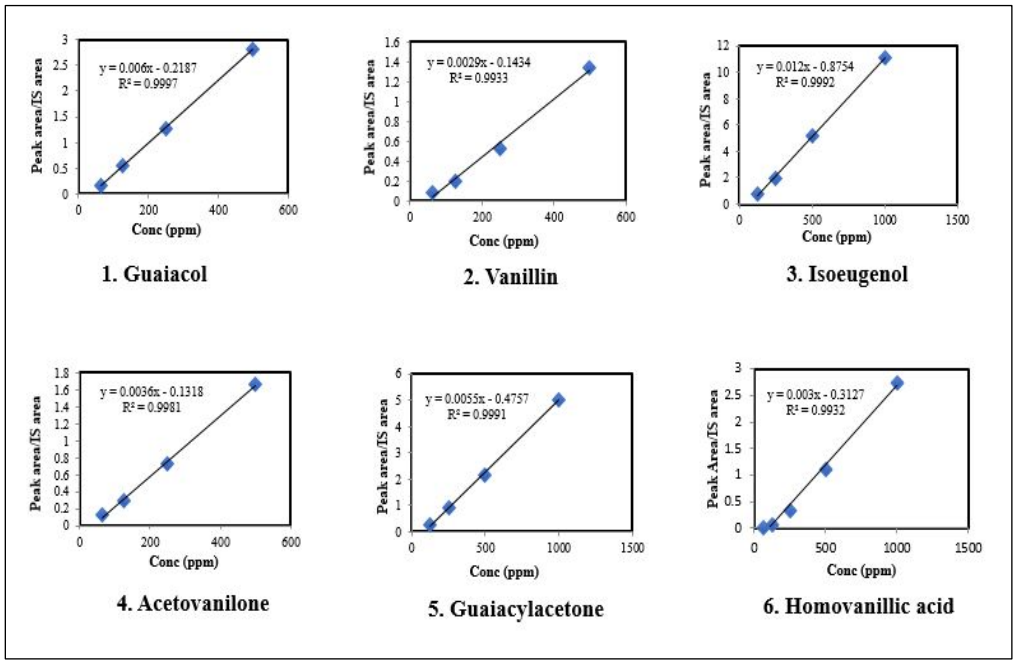

Figure S5. Calibration curves for standard phenolic monomers.

1. Kruse, A. and E. Dinjus, *Hot compressed water as reaction medium and reactant: properties and synthesis reactions.* The Journal of supercritical fluids, 2007. **39**(3): p. 362-380.
2. Krammer, P. and H. Vogel, *Hydrolysis of esters in subcritical and supercritical water.* The Journal of Supercritical Fluids, 2000. **16**(3): p. 189-206.