

ACTIVATED CARBON FROM WINEMAKING WASTE: THERMOECONOMIC ANALYSIS FOR LARGE SCALE PRODUCTION

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Supplementary

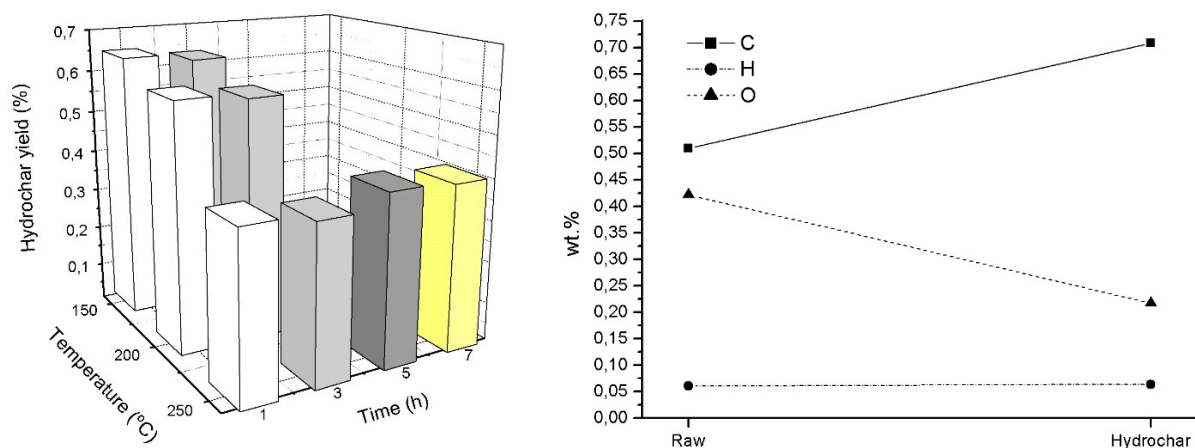


Figure S1. Solid yield of the HTC of vineyard pruning wood under experimental conditions (a) and elemental composition of raw and hydrochar after 1 hour of treatment (b).

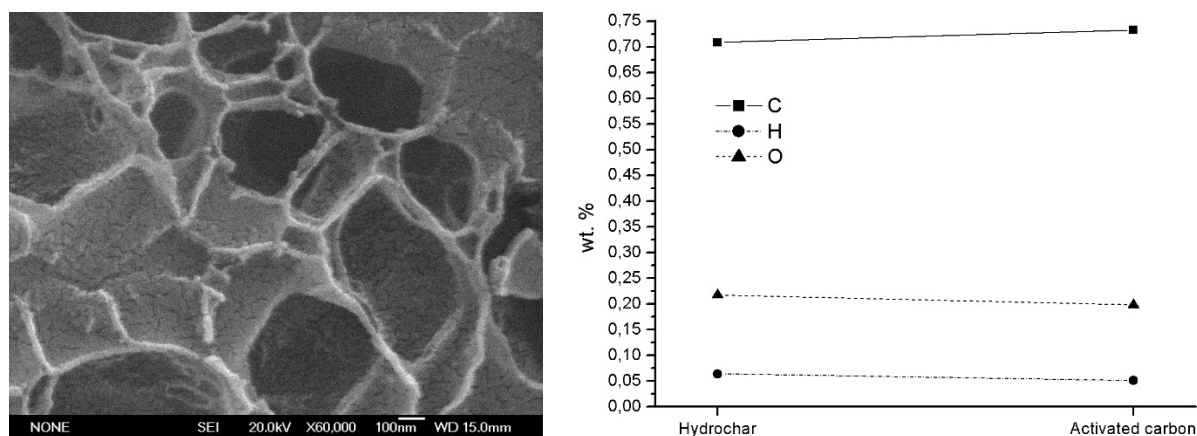


Figure S2. SEM image of the activated carbon porous structure obtained (a) and variation on the elemental composition during the activation treatment (b).

Table S1. Mass balance of Hydrothermal Carbonization.

Compounds	Mass (g)
Vineyard pruning wood	10.0
Water	135.0
Hydrochar	4.0
Aqueous phase	136.45
Gas	4.55

Table S2. Non-condensable phase composition detected by GC-MS.

Compound	wt. %
2-Furancarboxaldehyde, 5-(hydroxymethyl) [$C_6H_6O_3$]	8,90
2-Furancarboxaldehyde [$C_5H_4O_2$]	7,16
Phosphine oxide, trioctyl- [$C_{24}H_{50}O_3P$]	6,19
1,2-Benzenediol [$C_6H_6O_2$]	5,88
2-Furancarboxaldehyde, 5-methyl- [$C_6H_6O_2$]	5,84
Phenol [C_6H_6O]	3,93
1,2-Cyclopentanedione,3-methyl- [$C_6H_8O_2$]	3,48
Phenol, 2-methoxy- [$C_7H_8O_2$]	2,83
Benzoic acid [$C_7H_6O_2$]	2,80
1,3-Benzenediol, 2-methyl- [$C_7H_8O_2$]	2,29
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- [$C_{10}H_{12}O_3$]	2,23
1,3-Pentanediol, 2,2,4-trimethyl [$C_{12}H_{26}O_4$]	1,87
Phenol, 2,6-dimethoxy- [$C_8H_{10}O_3$]	1,84
Benzenemethanol, 4-hydroxy- [$C_7H_8O_2$]	1,58
Benzaldehyde, 4-hydroxy-3-methoxy- [$C_8H_8O_3$]	1,56
2-Decyn-1-ol [$C_{10}H_{18}O$]	1,54
Cyclopentan-1-al, 4-isopropylidene-2-methyl- [$C_{10}H_{16}O$]	1,50
Cyclopentylcarboxylic acid [$C_6H_{10}O_2$]	1,42
Benzene, 1,4-dimethoxy-2-methyl- [$C_9H_{12}O_2$]	1,33
trans-.beta.-Terpinyl pentanoate [$C_{15}H_{26}O_2$]	1,31
3-ethyl-2-hydroxy-2-cyclopenten-1-one [$C_7H_{10}O_2$]	1,27
Cis-limonene oxide [$C_{10}H_{16}O$]	1,10
Pentanoic acid, 4-oxo- [$C_5H_8O_3$]	1,09
2-Methoxy-5-methylphenol [$C_8H_{10}O_2$]	1,07
2-cyclopenten-1-one, 2-hydroxy-3-methyl- [$C_6H_8O_2$]	1,02
Nicotinic acid, 2-amino-,hydrazide [$C_6H_8N_4O$]	1,02
1H-Indene-1,5(6H)-dione, 2,3,7,7a-tetrahydro-7a-methyl- [$C_{10}H_{12}O_2$]	0,89
3-methyl-phenol [C_7H_8O]	0,88
Adipic acid, ethyl 5-methoxy-3-methylpentyl ester [$C_6H_{10}O_4$]	0,87
Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- [$C_9H_{10}O_3$]	0,85
1-Undecanol [$C_{11}H_{24}O$]	0,82
2,3-Dimethylhydroquinone [$C_8H_{10}O_2$]	0,82
Benzyl oxy tridecanoic acid [$C_{20}H_{32}O_3$]	0,80
Tricyclo[4.2.1.1(2,5)]dec-3-en-9-one [$C_{10}H_{12}O$]	0,80
Ethanone, 1-(3-hydroxyphenyl) [$C_8H_8O_2$]	0,80

1-Pentadecene, 2-methyl- [C ₁₆ H ₃₂]	0,78
2-Undecenoic acid [C ₁₁ H ₂₀ O ₂]	0,76
3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-Tris(trimethylsiloxy)tetrasiloxane [C ₁₈ H ₅₂ O ₇ Si ₇]	0,75
2-Methoxy-4-vinylphenol [C ₉ H ₁₀ O ₂]	0,69
Cyclopentanol,1-ethyl- [C ₇ H ₁₄ O]	0,67
Acetic acid [C ₂ H ₄ O ₂]	0,63
5-Chlorovaleric acid [C ₅ H ₉ ClO ₂]	0,61
1H-Pyrrole-2-carboxaldehyde [C ₅ H ₅ NO]	0,61
p-Menthan-4-ol [C ₁₀ H ₂₀ O]	0,60
2-Decenal [C ₁₀ H ₁₈ O]	0,60
Hexanoic acid [C ₆ H ₁₂ O ₂]	0,56
2H-1-Benzopyran-2-one, 8-hydroxy- [C ₉ H ₆ O ₃]	0,56
2H-Pyran-2-one, 5,6-dihydro-3,5,5-trimethyl- [C ₈ H ₁₂ O ₂]	0,52
Bicyclo [4.3.0]nonan-2-one, 8-isopropylidene [C ₁₂ H ₁₈ O]	0,52
2,6-xyleneol [C ₈ H ₁₀ O]	0,51
2-Furanmethanol, 5-(2-furanylmethyl)- [C ₁₀ H ₁₀ O ₃]	0,51
Heptadecane [C ₁₇ H ₃₄]	0,50
2-Nonen-1-ol [C ₉ H ₁₈ O]	0,50
Cyclohexanol, dodecyl- [C ₁₈ H ₃₆ O]	0,49
2,5-Piperazinedione, 3,6-bis(2-methylpropyl)- [C ₁₂ H ₁₈ N ₄ O ₄]	0,46
2,2,5,5,6-Pentamethyl-4,7,9-trioxabicyclo[4.2.1]nonane [C ₁₁ H ₂₀ O ₃]	0,44
tert-Butyl ethyl malonate [C ₉ H ₁₆ O ₄]	0,44
1,6-Pentalenedione, hexahydro-6a-(2-propynyl)-,cis- [C ₈ H ₁₀ O ₂]	0,44
2-Butenoic acid, 2-methyl-, (Z)- [C ₅ H ₈ O ₂]	0,43
1-Decanol [C ₁₀ H ₂₂ O]	0,42
2-Cyclohexen-1-one, 2-hydroxy-3-methyl-6-(1-methylethyl)- [C ₁₀ H ₁₆ O ₂]	0,39
Nona-3,5-dien-2-one [C ₉ H ₁₄ O]	0,39
Cyclohexanone, 4-ethyl- [C ₈ H ₁₄ O]	0,38
Propanoic acid [C ₃ H ₆ O ₂]	0,38
Furan, 2,5-dimethyl- [C ₆ H ₈ O]	0,37
4-Dodecyne [C ₁₂ H ₂₂]	0,36
2,4-Heptadienal, (E,E)- [C ₇ H ₁₀ O]	0,35
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15 [C ₁₆ H ₄₈ O ₇ Si ₈]	0,34
n-Decanoic acid [C ₁₀ H ₂₀ O ₂]	0,34
3-ethylcyclopent-2-en-1-one [C ₇ H ₁₀ O]	0,30
2(3H)-Furanone, 5-heptyldihydro- [C ₁₁ H ₂₀ O ₂]	0,28
Dodecane, 2,6,10-trimethyl- [C ₁₅ H ₃₂]	0,22
Furan, 2,3,5-trimethyl- [C ₇ H ₁₀ O]	0,18
2-Cyclohexen-1-one, 2-hydroxy-6-methyl-3-(1-methylethyl)- [C ₁₀ H ₁₆ O ₂]	0,20
Phenol, 2-methoxy-3-(2-propenyl)- [C ₁₀ H ₁₂ O ₂]	0,17
Hexadecane [C ₁₆ H ₃₄]	0,17
Dodecane, 2-methyl- [C ₁₃ H ₂₈]	0,16
Octadecane [C ₁₈ H ₃₈]	0,16
Dodecane [C ₁₂ H ₂₆]	0,14
Indene-1,7(4H)-dione, 3a,7a-dihydro-5-methyl- [C ₁₀ H ₁₀]	0,14

7-Nonynoic acid [C ₉ H ₁₄ O ₂]	0,14
Tricosane [C ₂₃ H ₄₈]	0,14
1(2H)-Naphthalenone, 3,4,5,6,7,8- hexahydro- [C ₁₀ H ₁₄ O]	0,11
2-Propanone, 1-(acetyloxy)- [C ₅ H ₈ O ₃]	0,11
sulfurous acid, 2-ethylhexyl isohexyl ester [C ₁₄ H ₃₀ O ₃ S]	0,10
2,6-Octadiene, 1-methoxy-3,7-dimethyl- [C ₁₁ H ₂₀ O]	0,09
1-Methylcycloheptene [C ₈ H ₁₄]	0,09
1,4-Pentadiene, 3-propyl- [C ₈ H ₁₄]	0,05
3-Ethoxy-2-butanone [C ₆ H ₁₂ O ₂]	0,04
Butane, 2-ethoxy- [C ₆ H ₁₄ O]	0,04
Undecane [C ₁₁ H ₂₄]	0,03
2,3-Butanedione [C ₄ H ₆ O ₂]	0,02
2-Pentanone,3-methyl- [C ₆ H ₁₂ O]	0,02

Table S2. Elemental composition of the non-condensable organic phase analysed by GC-MS.

Element	wt. %
C	66.6
H	7.6
O	25.8

Table S4. Chemical composition of the HTC aqueous phase assumed for the process analysis.

Compounds	wt. %
Water	98.91
Furfural	0.52
Phenol	0.19
Adipic acid	0.09
1-undecanol	0.09
Acetic acid	0.05
Hexanoic acid	0.04
Heptadecane	0.03
1-decanol	0.03
Propanoic acid	0.03
n-decanoic acid	0.02

Table S5. Chemical composition estimated for the HTC gaseous phase.

Compounds	wt. %
CO ₂	87.00
CH ₄	4.54
H ₂	4.46
CO	4.00

Table S6. Mass balance of the activation.

Compounds	Mass (g)
Hydrochar	4.00
Steam	30.00
Activated carbon	2.44
Gas	31.56
Condensed	-

Table S7. Chemical composition estimated for the activation gas phase.

Compounds	wt.%
H ₂ O	90.72
CO	6.60
CO ₂	1.79
H ₂	0.90