processes

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Supplementary material

Comparative Technical Process and Product Assessment of Catalytic and Thermal Pyrolysis of Lignocellulosic Biomass

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Supporting information

Table S1. Output data from pyrolysis reactions used for process simulations.

	Formula	Cs/ASA	Na-alumina	HY-Zeolite	Thermal
CHAR+COKE		18.55	25.13	28.44	11.43
WATER	H_2O	32.06	29.12	33.04	21.51
Gaseous components		24.61	24.27	19.22	13.98
OXYGEN	O_2	0.00	0.00	0.00	0.00
NITROGEN	N_2	0.00	0.00	0.00	0.00
HYDROGEN	H_2	0.00	0.00	0.01	0.00
CARBON-MONOXIDE	CO	0.47	0.32	0.44	0.36
CARBON-DIOXIDE	CO_2	0.37	0.54	0.37	0.46
AMMONIA	H_3N	0.10	0.10	0.13	0.11
ARGON	AR	0.00	0.00	0.00	0.00
NITRIC-OXIDE	NO	0.00	0.00	0.00	0.00
NITROGEN-DIOXIDE	NO_2	0.00	0.00	0.00	0.00
CHLORINE	Cl_2	0.00	0.00	0.00	0.00
SULFUR-DIOXIDE	O_2S	0.01	0.01	0.02	0.02
METHANE	CH_4	0.02	0.02	0.02	0.02
ETHANE	C_2H_6	0.01	0.01	0.01	0.04
ETHYLENE	C_2H_4	0.00	0.00	0.00	0.00
PROPANE	C_3H_8	0.00	0.00	0.00	0.00
Organics		15.79	12.48	10.30	44.09
N-BUTANOL	$C_4H_{10}O$	3.38	0.00	0.00	0.82
CROTONALDEHYDE	C_4H_6O	0.00	2.36	3.59	2.61
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$	5.84	1.01	1.31	0.20
CYCLOPENTANONE	C_5H_8O	1.53	1.35	5.54	0.00

CYCLOPENTENONE	C_5H_6O	0.68	4.93	8.72	2.45
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	5.19	13.27	8.96	12.25
FORMIC-ACID	CH_2O_2	0.00	0.00	0.00	0.00
ACETIC-ACID	$C_2H_4O_2$	4.28	0.00	13.10	6.81
PROPIONIC-ACID	$C_3H_6O_2$	0.00	0.00	0.55	0.00
C6H10O5-N1	$C_6H_{10}O_5$	0.00	0.00	0.00	0.00
DEXTROSE	$C_6H_{12}O_6$	0.00	0.00	0.00	14.97
PHENOL	C_6H_6O	2.89	8.17	2.11	0.95
GUAIACOL	$C_7H_8O_2$	1.86	0.00	7.18	6.81
P-CRESOL	C_7H_8O	3.30	5.91	4.09	2.86
METHYL-PHENYL-KETONE	C_8H_8O	0.00	0.00	0.00	0.00
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	2.56	0.84	11.52	11.98
2,4-XYLENOL	$C_8H_{10}O$	4.02	5.39	3.00	1.22
VANILLIN	$C_8H_8O_3$	0.00	2.08	1.62	12.79
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	3.08	1.69	14.11	16.33
MESITYL-ALCOHOL	$C_9H_{12}O$	0.14	8.19	0.00	0.00
FURAN	C_4H_4O	24.82	3.80	0.00	0.00
FURFURAL	$C_5H_4O_2$	5.95	3.11	8.02	3.54
5-METHYLFURFURAL	$C_6H_6O_2$	3.62	1.37	2.75	3.13
1-PENTENE	C_5H_{10}	2.90	0.59	0.00	0.00
N-OCTANE	C_8H_{18}	2.76	1.74	0.00	0.00
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	0.00	0.00	0.00	0.00
N-DECANE	$C_{10}H_{22}$	1.80	0.00	0.00	0.00
N-HEXADECANE	$C_{16}H_{34}$	7.05	0.00	0.00	0.00
TOLUENE	C_7H_8	1.13	0.00	0.70	0.00
O-XYLENE	C_8H_{10}	0.83	7.19	0.00	0.00
ETHYLBENZENE	C_8H_{10}	0.72	5.18	0.93	0.00
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	0.22	0.00	0.70	0.00
INDENE	C_9H_8	1.11	1.52	0.42	0.00
NAPHTHALENE	$C_{10}H_8$	2.40	3.36	0.00	0.00
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	1.71	1.94	0.00	0.00
2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	0.11	0.61	0.00	0.00
PHENANTHRENE	$C_{14}H_{10}$	0.00	0.00	0.00	0.00
RETENE	$C_{18}H_{18}$	0.00	0.62	0.00	0.27
BENZENE	C_6H_6	0.59	6.91	1.07	0.00
2-METHYLBENZOFURAN	C_9H_8O	2.06	2.90	0.00	0.00
COUMARONE	C_8H_6O	1.45	3.97	0.00	0.00

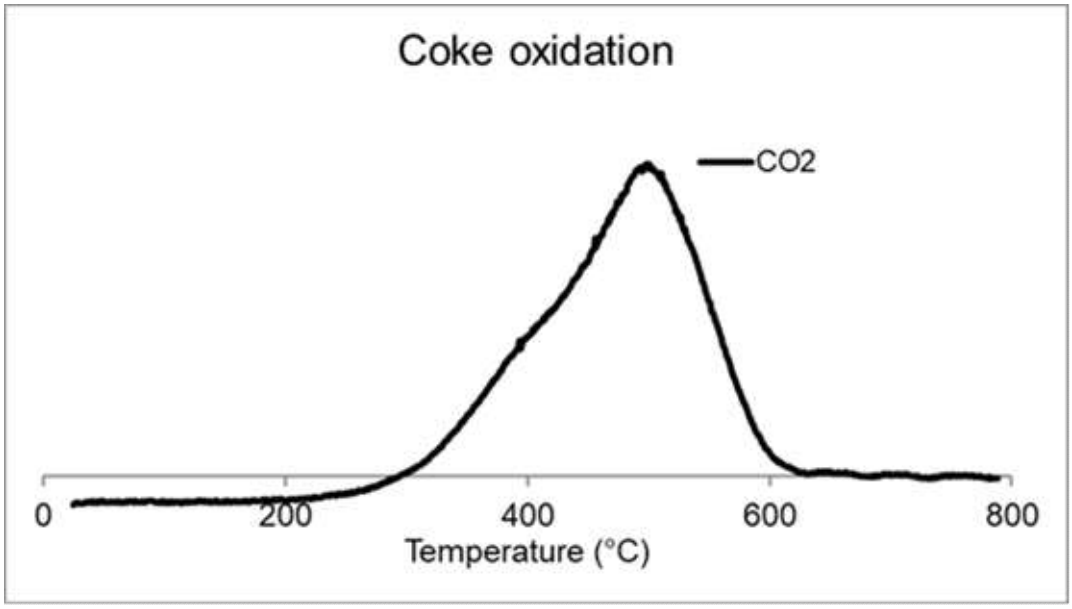

Figure S1. Temperature-programmed oxidation of coke formed on the Cs/ASA catalyst.

Table S2. Data and assumptions for separation model.

	Formula	CAS no.	Log Kow	Aqueous stream fraction	Organic stream fraction
N-BUTANOL	$C_4H_{10}O$	71-36-3	0.84	0.95	0.05
CROTONALDEHYDE	C_4H_6O	004170-30-3	0.6	0.95	0.05
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$	107-87-9	0.91	0.95	0.05
CYCLOPENTANONE	C_5H_8O	120-92-3	0.63	0.95	0.05
CYCLOPENTENONE	C_5H_6O	930-30-3	0.71	0.95	0.05
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	001120-73-6	1.26	0.95	0.05
FORMIC-ACID	CH_2O_2	64-18-6	-0.54	0.95	0.05
ACETIC-ACID	$C_2H_4O_2$	64-19-7	-0.17	0.95	0.05
PROPIONIC-ACID	$C_3H_6O_2$	79-09-4	0.33	0.95	0.05
C6H10O5-N1	$C_6H_{10}O_5$	498-07-7	-1.25	0.95	0.05
DEXTROSE	$C_6H_{12}O_6$	2595-97-3	-3.24	0.95	0.05
PHENOL	C_6H_6O	108-95-2	1.46	0.05	0.95
GUAIACOL	$C_7H_8O_2$	90-05-1	1.32	0.95	0.05
P-CRESOL	C_7H_8O	106-44-5	1.94	0.05	0.95
METHYL-PHENYL-KETONE	C_8H_8O	98-86-2	1.58	0.05	0.95
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	93-51-6	1.88	0.05	0.95
2,4-XYLENOL	$C_8H_{10}O$	105-67-9	2.3	0.05	0.95
VANILLIN	$C_8H_8O_3$	121-33-5	1.21	0.95	0.05
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	89-72-5	3.27	0.05	0.95
MESITYL-ALCOHOL	$C_9H_{12}O$	527-60-6	2.73	0.05	0.95
FURAN	C_4H_4O	110-00-9	1.34	0.05	0.95
FURFURAL	$C_5H_4O_2$	98-01-1	0.41	0.95	0.05
5-METHYLFURFURAL	$C_6H_6O_2$	620-02-0	0.67	0.95	0.05
1-PENTENE	C_5H_{10}	109-67-1	2.66	0.05	0.95
N-OCTANE	C_8H_{18}	111-65-9	5.18	0.05	0.95
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	540-84-1	5.83	0.05	0.95
N-DECANE	$C_{10}H_{22}$	124-18-5	5.01	0.05	0.95
N-HEXADECANE	$C_{16}H_{34}$	544-76-3	8.2	0.05	0.95
TOLUENE	C_7H_8	108-88-3	2.73	0.05	0.95
O-XYLENE	C_8H_{10}	95-47-6	3.12	0.05	0.95
ETHYLBENZENE	C_8H_{10}	100-41-4	3.15	0.05	0.95
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	95-63-6	3.63	0.05	0.95
INDENE	C_9H_8	95-13-6	2.92	0.05	0.95
NAPHTHALENE	$C_{10}H_8$	91-20-3	3.3	0.05	0.95
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	91-57-6	3.86	0.05	0.95

2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	581-42-0	4.31	0.05	0.95
PHENANTHRENE	$C_{14}H_{10}$	85-01-8	4.46	0.05	0.95
RETENE	$C_{18}H_{18}$	483-65-8	6.35	0.05	0.95
BENZENE	C_6H_6	71-43-2	2.13	0.05	0.95
2-METHYLBENZOFURAN	C_9H_8O	004265-25-2	3.22	0.05	0.95
COUMARONE	C_8H_6O	271-89-6	2.67	0.05	0.95
Water	H_2O			0.95	0.05

Table S3. Key stream names and descriptions for the streams reported in tables S4-S7.

Stream name	**Description**
Pyro-In	Feed stream entering the process
Pyro-Out	Stream coming out of the Pyrolyzer
GASBIO	Stream coming out of cyclone separators and containing gas and bio-oil
LitStr	Light stream after separation of heavy oil in Flash 1
PyGas	Gaseous stream after gas separation in Flash 2
WatOil	Oil stream after gas separation in Flash 2 and input to Phase sep 1
OrgOil	Oil stream going to distillation after phase separation
AqOil	Aqueous stream going to hydrogen production after phase separation
DistAq	Distillate going to mixing with AqOil and hydrogen production
H2Prod	Outlet stream from hydrogen production
DO-Oil	Product oil stream from distillation bottoms

Table S4. Stream flow data for pyrolysis using Cs/ASA catalyst.

Stream		Pyro-In	Pyro-Out	GasBio	LitStr	PyGas	WatOil	OrgOil	AqOil	DistAq	H2Prod	DO-Oil
Total mass flow		21000	21000.1	15490.9	14448.8	6336.4	8112.4	1458.8	6653.6	766.2	7419.9	684.9
PINEWOOD		20000										
CHAR			3709.2									
ASH			1800.0									
WATER	H_2O		6411.1	6411.1	6411.1	118.6	6292.5	314.6	5977.9	314.4	4301.6	0.0
OXYGEN	O_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN	N_2	1000	1000.0	1000.0	1000.0	1000.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	H_2		22.0	22.0	22.0	22.0	0.0	0.0	0.0	0.0	308.1	0.0
CARBON-MONOXIDE	CO		2323.9	2323.9	2323.9	2323.8	0.1	0.1	0.1	0.0	0.0	0.0
CARBON-DIOXIDE	CO_2		1843.7	1843.7	1843.7	1841.1	2.6	1.3	1.3	0.1	2810.2	0.0
AMMONIA	H_3N		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	AR		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITRIC-OXIDE	NO		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN-DIOXIDE	NO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHLORINE	Cl_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SULFUR-DIOXIDE	SO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHANE	CH_4		501.4	501.4	501.4	499.0	2.4	1.2	1.2	0.3	0.0	0.0
ETHANE	C_2H_6		64.2	64.2	64.2	61.5	2.8	1.4	1.4	1.0	0.0	0.0
ETHYLENE	C_2H_4		99.7	99.7	99.7	97.1	2.6	1.3	1.3	0.8	0.0	0.0
PROPANE	C_3H_8		67.0	67.0	67.0	55.9	11.0	5.5	5.5	5.0	0.0	0.0
N-BUTANOL	$C_4H_{10}O$		113.3	113.3	75.9	3.0	72.9	3.6	69.2	3.6	0.0	0.0
CROTONALDEHYDE	C_4H_6O		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$		195.6	195.6	131.1	69.3	61.8	3.1	58.7	3.1	0.0	0.0

CYCLOPENTANONE	C_5H_8O	51.3	51.3	34.4	5.7	28.7	1.4	27.2	1.4	0.0	0.0
CYCLOPENTENONE	C_5H_6O	22.7	22.7	15.2	0.2	15.0	0.8	14.3	0.5	0.0	0.2
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	173.9	173.9	116.5	0.2	116.3	5.8	110.5	0.0	0.0	5.8
FORMIC-ACID	CH_2O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC-ACID	$C_2H_4O_2$	143.4	143.4	96.0	1.1	95.0	4.8	90.2	4.7	0.0	0.0
PROPIONIC-ACID	$C_3H_6O_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C6H10O5-N1	$C_6H_{10}O_5$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DEXTROSE	$C_6H_{12}O_6$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENOL	C_6H_6O	96.6	96.6	64.8	0.3	64.5	61.2	3.2	7.0	0.0	54.2
GUAIACOL	$C_7H_8O_2$	62.4	62.4	41.8	0.0	41.8	2.1	39.7	0.0	0.0	2.1
P-CRESOL	C_7H_8O	110.5	110.5	74.0	0.2	73.8	70.1	3.7	0.0	0.0	70.1
METHYL-PHENYL-KETONE	C_8H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	85.5	85.5	57.3	0.0	57.3	54.4	2.9	0.0	0.0	54.4
2,4-XYLENOL	$C_8H_{10}O$	134.6	134.6	90.2	0.0	90.2	85.6	4.5	0.0	0.0	85.6
VANILLIN	$C_8H_8O_3$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	103.1	103.1	69.1	0.0	69.1	65.6	3.5	0.0	0.0	65.6
MESITYL-ALCOHOL	$C_9H_{12}O$	4.6	4.6	3.1	0.0	3.1	2.9	0.2	0.0	0.0	2.9
FURAN	C_4H_4O	831.0	831.0	556.8	166.4	390.4	370.9	19.5	367.4	0.0	0.0
FURFURAL	$C_5H_4O_2$	199.3	199.3	133.5	7.2	126.4	6.3	120.0	5.0	0.0	1.3
5-METHYLFURFURAL	$C_6H_6O_2$	121.2	121.2	81.2	0.0	81.1	4.1	77.1	0.0	0.0	4.1
1-PENTENE	C_5H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-OCTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-DECANE	$C_{10}H_{22}$	60.1	60.1	40.3	9.5	30.8	29.3	1.5	29.2	0.0	0.0
N-HEXADECANE	$C_{16}H_{34}$	235.8	235.8	158.0	0.0	158.0	150.1	7.9	0.0	0.0	150.1
TOLUENE	C_7H_8	37.9	37.9	25.4	20.7	4.7	4.5	0.2	4.3	0.0	0.0

O-XYLENE	C_8H_{10}	27.7	27.7	18.6	9.7	8.8	8.4	0.4	8.3	0.0	0.0
ETHYLBENZENE	C_8H_{10}	24.0	24.0	16.1	10.2	5.9	5.6	0.3	5.5	0.0	0.0
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	7.4	7.4	5.0	1.3	3.7	3.5	0.2	3.5	0.0	0.0
INDENE	C_9H_8	37.0	37.0	24.8	0.0	24.8	23.5	1.2	0.0	0.0	23.5
NAPHTHALENE	$C_{10}H_8$	80.5	80.5	53.9	0.0	53.9	51.2	2.7	0.0	0.0	51.2
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	57.3	57.3	38.4	0.0	38.4	36.5	1.9	0.0	0.0	36.5
2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	3.7	3.7	2.5	0.0	2.5	2.4	0.1	0.0	0.0	2.4
PHENANTHRENE	$C_{14}H_{10}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RETENE	$C_{18}H_{18}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BENZENE	C_6H_6	19.9	19.9	13.3	12.3	1.0	0.9	0.0	0.9	0.0	0.0
2-METHYLBENZOFURAN	C_9H_8O	68.9	68.9	46.2	0.0	46.1	43.8	2.3	0.0	0.0	43.8
COUMARONE	C_8H_6O	48.6	48.6	32.5	0.0	32.5	30.9	1.6	0.0	0.0	30.9
Temperature (Deg Celsius)		450.0	450.0	280.0	25.0	25.0	25.0	25.0	40.0	600.0	30.0
Pressure (bar)		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	13.7	1.0

Table S5. Stream flow data for pyrolysis using Na-Alumina catalyst.

Stream		Pyro-In	Pyro-Out	GasBio	LitStr	PyGas	WatOil	OrgOil	AqOil	DistAq	H2Prod	DO-Oil
Total mass flow		21000	21000.1	14174.1	13350.5	6224.5	7126.0	1180.4	5945.6	406.0	6351.5	730.7
PINEWOOD		20000										
CHAR			5026.0									
ASH			1800.0									
WATER	H_2O		5823.4	5823.4	5823.4	108.9	5714.5	285.7	5428.8	284.7	4437.6	0.0
OXYGEN	O_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN	N_2	1000	1000.0	1000.0	1000.0	1000.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	H_2		8.5	8.5	8.5	8.5	0.0	0.0	0.0	0.0	192.2	0.0
CARBON-MONOXIDE	CO		1535.8	1535.8	1535.8	1535.8	0.1	0.0	0.0	0.0	0.0	0.0
CARBON-DIOXIDE	CO_2		2602.4	2602.4	2602.4	2599.2	3.2	1.6	1.6	0.0	1721.7	0.0
AMMONIA	H_3N		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	AR		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITRIC-OXIDE	NO		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN-DIOXIDE	NO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHLORINE	Cl_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SULFUR-DIOXIDE	SO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHANE	CH_4		490.6	490.6	490.6	488.3	2.4	1.2	1.2	0.1	0.0	0.0
ETHANE	C_2H_6		66.1	66.1	66.1	63.3	2.8	1.4	1.4	0.7	0.0	0.0
ETHYLENE	C_2H_4		89.6	89.6	89.6	87.3	2.3	1.2	1.2	0.4	0.0	0.0
PROPANE	C_3H_8		61.9	61.9	61.9	51.7	10.1	5.1	5.1	4.0	0.0	0.0
N-BUTANOL	$C_4H_{10}O$		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CROTONALDEHYDE	C_4H_6O		60.4	60.4	40.5	1.1	39.4	2.0	37.4	2.0	0.0	0.0
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$		25.9	25.9	17.3	9.7	7.6	0.4	7.2	0.3	0.0	0.0
CYCLOPENTANONE	C_5H_8O		34.5	34.5	23.1	4.4	18.7	0.9	17.8	0.9	0.0	0.0

CYCLOPENTENONE	C_5H_6O	126.0	126.0	84.4	1.0	83.4	4.2	79.2	4.1	0.0	0.1
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	339.1	339.1	227.2	0.4	226.8	11.3	215.5	0.0	0.0	11.3
FORMIC-ACID	CH_2O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC-ACID	$C_2H_4O_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROPIONIC-ACID	$C_3H_6O_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C6H10O5-N1	$C_6H_{10}O_5$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DEXTROSE	$C_6H_{12}O_6$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENOL	C_6H_6O	208.8	208.8	139.9	0.7	139.2	132.2	7.0	16.9	0.0	115.8
GUAIACOL	$C_7H_8O_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
P-CRESOL	C_7H_8O	151.0	151.0	101.2	0.4	100.8	95.8	5.0	0.0	0.0	95.8
METHYL-PHENYL-KETONE	C_8H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	21.6	21.6	14.5	0.0	14.5	13.7	0.7	0.0	0.0	13.7
2,4-XYLENOL	$C_8H_{10}O$	137.6	137.6	92.2	0.0	92.2	87.6	4.6	0.0	0.0	87.6
VANILLIN	$C_8H_8O_3$	53.1	53.1	35.6	0.0	35.6	1.8	33.8	0.0	0.0	1.8
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	43.1	43.1	28.9	0.0	28.9	27.5	1.4	0.0	0.0	27.5
MESITYL-ALCOHOL	$C_9H_{12}O$	209.2	209.2	140.2	0.0	140.2	133.2	7.0	0.0	0.0	133.2
FURAN	C_4H_4O	97.1	97.1	65.0	19.5	45.5	43.2	2.3	42.0	0.0	0.0
FURFURAL	$C_5H_4O_2$	79.4	79.4	53.2	2.8	50.4	2.5	47.9	1.8	0.0	0.7
5-METHYLFURFURAL	$C_6H_6O_2$	34.9	34.9	23.4	0.0	23.4	1.2	22.2	0.0	0.0	1.2
1-PENTENE	C_5H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-OCTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-DECANE	$C_{10}H_{22}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-HEXADECANE	$C_{16}H_{34}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOLUENE	C_7H_8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O-XYLENE	C_8H_{10}	183.8	183.8	123.1	69.9	53.2	50.6	2.7	31.5	0.0	0.0

ETHYLBENZENE	C_8H_{10}	132.4	132.4	88.7	60.7	28.1	26.7	1.4	14.5	0.0	0.0
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
INDENE	C_9H_8	38.8	38.8	26.0	0.0	26.0	24.7	1.3	0.0	0.0	24.7
NAPHTHALENE	$C_{10}H_8$	85.9	85.9	57.5	0.0	57.5	54.6	2.9	0.0	0.0	54.6
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	49.6	49.6	33.2	0.0	33.2	31.6	1.7	0.0	0.0	31.6
2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	15.5	15.5	10.4	0.0	10.4	9.9	0.5	0.0	0.0	9.9
PHENANTHRENE	$C_{14}H_{10}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RETENE	$C_{18}H_{18}$	16.0	16.0	10.7	0.0	10.7	10.2	0.5	0.0	0.0	10.2
BENZENE	C_6H_6	176.4	176.4	118.2	110.9	7.3	6.9	0.4	1.9	0.0	0.0
2-METHYLBENZOFURAN	C_9H_8O	74.2	74.2	49.7	0.0	49.7	47.2	2.5	0.0	0.0	47.2
COUMARONE	C_8H_6O	101.4	101.4	67.9	0.1	67.8	64.5	3.4	0.0	0.0	64.5
Temperature (Deg Celsius)		450.0	450.0	280.0	25.0	25.0	25.0	25.0	45.0	600.0	30.0
Pressure (bar)		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	13.7	1.0

Table S6. Stream flow data for pyrolysis using HY-Zeolite catalyst.

Stream		Pyro-In	Pyro-Out	GasBio	LitStr	PyGas	WatOil	OrgOil	AqOil	DistAq	H2Prod	DO-Oil
Total mass flow		21000	21000.1	0.0	12831.4	5002.0	7829.5	839.8	6989.6	360.3	7349.9	474.5
PINEWOOD		20000										
CHAR			5689.0									
ASH			1800.0									
WATER	H_2O		6608.0		6608.0	99.2	6508.7	325.4	6183.3	325.2	5185.9	0.0
OXYGEN	O_2		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN	N_2	1000	1000.0		1000.0	1000.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	H_2		21.1		21.1	21.1	0.0	0.0	0.0	0.0	209.1	0.0
CARBON-MONOXIDE	CO		1697.1		1697.1	1697.0	0.1	0.0	0.0	0.0	0.0	0.0
CARBON-DIOXIDE	CO_2		1411.5		1411.5	1409.5	2.0	1.0	1.0	0.1	1954.9	0.0
AMMONIA	H_3N		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	AR		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITRIC-OXIDE	NO		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN-DIOXIDE	NO_2		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHLORINE	Cl_2		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SULFUR-DIOXIDE	SO_2		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHANE	CH_4		491.6		491.6	488.7	2.9	1.4	1.4	0.3	0.0	0.0
ETHANE	C_2H_6		81.9		81.9	77.7	4.2	2.1	2.1	1.4	0.0	0.0
ETHYLENE	C_2H_4		93.6		93.6	90.7	2.9	1.5	1.5	0.8	0.0	0.0
PROPANE	C_3H_8		46.8		46.8	37.8	9.0	4.5	4.5	4.0	0.0	0.0
N-BUTANOL	$C_4H_{10}O$		0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CROTONALDEHYDE	C_4H_6O		73.9		49.5	1.1	48.4	2.4	46.0	2.4	0.0	0.0
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$		26.9		18.1	10.4	7.7	0.4	7.3	0.4	0.0	0.0

CYCLOPENTANONE	C_5H_8O	114.2	76.5	14.4	62.1	3.1	59.0	3.1	0.0	0.0
CYCLOPENTENONE	C_5H_6O	179.7	120.4	1.2	119.2	6.0	113.2	5.9	0.0	0.0
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	184.6	123.7	0.2	123.5	6.2	117.3	0.0	0.0	6.2
FORMIC-ACID	CH_2O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC-ACID	$C_2H_4O_2$	269.8	180.7	1.6	179.1	9.0	170.1	9.0	0.0	0.0
PROPIONIC-ACID	$C_3H_6O_2$	11.4	7.6	0.0	7.6	0.4	7.3	0.3	0.0	0.1
C6H10O5-N1	$C_6H_{10}O_5$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DEXTROSE	$C_6H_{12}O_6$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENOL	C_6H_6O	43.5	29.1	0.1	29.0	27.5	1.4	3.1	0.0	24.5
GUAIACOL	$C_7H_8O_2$	147.8	99.0	0.0	99.0	5.0	94.1	0.0	0.0	5.0
P-CRESOL	C_7H_8O	84.3	56.5	0.2	56.3	53.4	2.8	0.0	0.0	53.4
METHYL-PHENYL-KETONE	C_8H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	237.3	159.0	0.0	159.0	151.0	7.9	0.0	0.0	151.0
2,4-XYLENOL	$C_8H_{10}O$	61.7	41.4	0.0	41.3	39.3	2.1	0.0	0.0	39.3
VANILLIN	$C_8H_8O_3$	33.3	22.3	0.0	22.3	1.1	21.2	0.0	0.0	1.1
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	290.6	194.7	0.0	194.7	185.0	9.7	0.0	0.0	185.0
MESITYL-ALCOHOL	$C_9H_{12}O$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURAN	C_4H_4O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	$C_5H_4O_2$	165.2	110.7	5.5	105.2	5.3	99.9	3.7	0.0	1.5
5-METHYLFURFURAL	$C_6H_6O_2$	56.6	37.9	0.0	37.9	1.9	36.0	0.0	0.0	1.9
1-PENTENE	C_5H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-OCTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-DECANE	$C_{10}H_{22}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-HEXADECANE	$C_{16}H_{34}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOLUENE	C_7H_8	14.5	9.7	9.5	0.2	0.2	0.0	0.1	0.0	0.0

O-XYLENE	C_8H_{10}	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHYLBENZENE	C_8H_{10}	19.1		12.8	12.5	0.3	0.3	0.0	0.1	0.0	0.0
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	14.5		9.7	9.0	0.7	0.7	0.0	0.4	0.0	0.0
INDENE	C_9H_8	8.7		5.8	0.0	5.8	5.5	0.3	0.0	0.0	5.5
NAPHTHALENE	$C_{10}H_8$	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENANTHRENE	$C_{14}H_{10}$	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RETENE	$C_{18}H_{18}$	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BENZENE	C_6H_6	22.0		14.8	14.5	0.2	0.2	0.0	0.1	0.0	0.0
2-METHYLBENZOFURAN	C_9H_8O	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
COUMARONE	C_8H_6O	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature (Deg Celsius)		450.0	450.0	280.0	25.0	25.0	25.0	25.0	40.0	600.0	30.0
Pressure (bar)		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	13.7	1.0

Table S7. Stream flow data for thermal pyrolysis.

Stream		Pyro-In	Pyro-Out	GasBio	LitStr	PyGas	WatOil	OrgOil	AqOil	DistAq	H2Prod	DO-Oil
Total mass flow		21000	21000.1	16914.0	14268.9	3845.7	10423.2	2450.4	8944.7	279.3	12539.9	2140.7
PINEWOOD		20000										
CHAR			2286.0									
ASH			1800.0									
WATER	H_2O		4301.1	4301.1	4301.1	61.4	4239.7	260.6	4951.0	240.9	2835.9	0.0
OXYGEN	O_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN	N_2	1000	1000.0	1000.0	1000.0	1000.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	H_2		5.0	5.0	5.0	5.0	0.0	0.0	0.0	0.0	909.9	0.0
CARBON-MONOXIDE	CO		1001.1	1001.1	1001.1	1001.1	0.1	0.0	0.0	0.0	0.0	0.0
CARBON-DIOXIDE	CO_2		1276.5	1276.5	1276.5	1274.1	2.3	1.2	1.2	0.0	8794.2	0.0
AMMONIA	H_3N		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	AR		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITRIC-OXIDE	NO		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NITROGEN-DIOXIDE	NO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHLORINE	Cl_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SULFUR-DIOXIDE	SO_2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHANE	CH_4		300.3	300.3	300.3	298.4	1.9	1.0	1.0	0.0	0.0	0.0
ETHANE	C_2H_6		50.1	50.1	50.1	47.3	2.8	1.4	1.4	0.3	0.0	0.0
ETHYLENE	C_2H_4		62.6	62.6	62.6	60.5	2.1	1.1	1.1	0.2	0.0	0.0
PROPANE	C_3H_8		100.1	100.1	100.1	79.6	20.6	10.3	10.3	5.3	0.0	0.0
N-BUTANOL	$C_4H_{10}O$		72.0	72.0	50.4	1.0	49.4	2.5	46.9	2.1	0.0	0.0
CROTONALDEHYDE	C_4H_6O		230.4	230.4	161.3	3.2	158.1	7.9	150.2	3.3	0.0	4.6
METHYL-N-PROPYL-KETONE	$C_5H_{10}O$		18.0	18.0	12.6	3.7	8.9	0.4	8.4	0.2	0.0	0.0

CYCLOPENTANONE	C_5H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYCLOPENTENONE	C_5H_6O	216.0	216.0	151.2	1.4	149.9	7.5	142.4	0.0	0.0	7.5
2-METHYL-2-CYCLOPENTEN-1-ONE	C_6H_8O	1080.1	1080.1	756.1	1.0	755.1	37.8	717.3	0.0	0.0	37.8
FORMIC-ACID	CH_2O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC-ACID	$C_2H_4O_2$	600.1	600.1	420.0	3.5	416.5	20.8	395.7	0.1	0.0	20.7
PROPIONIC-ACID	$C_3H_6O_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C6H10O5-N1	$C_6H_{10}O_5$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DEXTROSE	$C_6H_{12}O_6$	1320.1	1320.1	924.1	0.0	924.1	46.2	877.9	0.0	0.0	46.2
PHENOL	C_6H_6O	84.0	84.0	58.8	0.1	58.7	55.8	2.9	16.9	0.0	38.7
GUAIACOL	$C_7H_8O_2$	600.1	600.1	420.0	0.0	420.0	21.0	399.0	0.0	0.0	21.0
P-CRESOL	C_7H_8O	252.0	252.0	176.4	0.1	176.3	167.5	8.8	0.4	0.0	167.1
METHYL-PHENYL-KETONE	C_8H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4-METHYL-2-METHOXYPHENOL	$C_8H_{10}O_2$	1056.1	1056.1	739.3	0.0	739.2	702.3	37.0	0.0	0.0	702.3
2,4-XYLENOL	$C_8H_{10}O$	108.0	108.0	75.6	0.0	75.6	71.8	3.8	0.0	0.0	71.8
VANILLIN	$C_8H_8O_3$	1128.1	1128.1	789.7	0.0	789.7	39.5	750.2	0.0	0.0	39.5
PHENOL,-O-SEC-BUTYL-	$C_{10}H_{14}O$	1440.1	1440.1	1008.1	0.1	1008.0	957.6	50.4	0.0	0.0	957.6
MESITYL-ALCOHOL	$C_9H_{12}O$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURAN	C_4H_4O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	$C_5H_4O_2$	312.0	312.0	218.4	4.1	214.3	10.7	203.6	9.6	0.0	0.4
5-METHYLFURFURAL	$C_6H_6O_2$	276.0	276.0	193.2	0.1	193.2	9.7	183.5	0.0	0.0	9.7
1-PENTENE	C_5H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-OCTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,2,4-TRIMETHYLPENTANE	C_8H_{18}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-DECANE	$C_{10}H_{22}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N-HEXADECANE	$C_{16}H_{34}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOLUENE	C_7H_8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

O-XYLENE	C_8H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHYLBENZENE	C_8H_{10}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1,2,4-TRIMETHYLBENZENE	C_9H_{12}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
INDENE	C_9H_8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NAPHTHALENE	$C_{10}H_8$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2-METHYLNAPHTHALENE	$C_{11}H_{10}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2,6-DIMETHYLNAPHTHALENE	$C_{12}H_{12}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHENANTHRENE	$C_{14}H_{10}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RETENE	$C_{18}H_{18}$	24.0	24.0	16.8	0.0	16.8	16.0	0.8	0.0	0.0	16.0
BENZENE	C_6H_6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2-METHYLBENZOFURAN	C_9H_8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
COUMARONE	C_8H_6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature (Deg Celsius)		450.0	450.0	280.0	25.0	25.0	25.0	25.0	79.3	600.0	30.0
Pressure (bar)		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	13.7	1.0

Table S8. Data values for figure 4 in the article.

	DO_oil				SH_oil/SC_oil				HT_oil			
	Cs/ASA	**Na-alumina**	**HY-Zeolite**	**Thermal**	**Cs/ASA**	**Na-alumina**	**HY-Zeolite**	**Thermal**	**Cs/ASA**	**Na-alumina**	**HY-Zeolite**	**Thermal**
Oxygen content (wt%)	7.90	10.80	15.90	17.30	7.58	10.49	15.45	15.09	3.70	3.70	3.70	3.70
Higher heating value (MJ/kg)	41.05	37.19	34.86	34.28	41.29	37.45	35.22	35.89	44.19	42.44	44.01	44.48
H/C molar ratio	1.45	1.15	1.28	1.32	1.45	1.15	1.29	1.36	1.51	1.26	1.48	1.55
O/C molar ratio	0.07	0.10	0.16	0.17	0.07	0.10	0.15	0.15	0.03	0.03	0.03	0.03
Oil yield (kg/kg biomass) %	3.42	3.65	2.37	10.70	3.35	3.57	2.32	10.32	3.25	3.39	2.11	9.42
H2 export yield (kg/kg biomass) %	1.54	0.96	1.05	4.55	1.54	0.96	1.04	4.46	1.49	0.86	0.94	4.00
Energy yield in oil (MJ/MJ biomass)%	8.04	7.77	4.73	20.99	7.91	7.65	4.67	21.18	8.22	8.23	5.32	23.97
Energy yield in H2 (MJ/MJ biomass)%	12.50	7.80	8.48	36.91	12.46	7.76	8.45	36.19	12.06	7.01	7.60	32.48