Supporting Information

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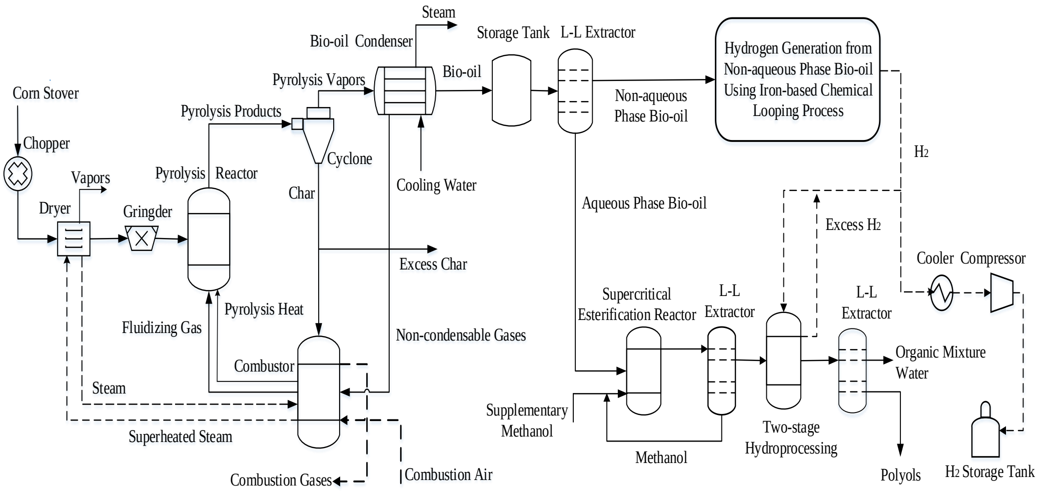

Figure S1. Process diagram for polyol and hydrogen production from corn stover via fast pyrolysis and upgrading

Table S1. Ultimate analysis, proximate analysis and lower calorific value of corn stover

1. Ultimate analysis (dry basis)	
Element	Value (wt. %)
Ash	6.23
Carbon	44.33
Hydrogen	5.73
Nitrogen	0.78
Chlorine	0.00
Sulphur	0.13
Oxygen	42.80
2. Proximate analysis(wet basis)	
Element	Value (wt. %)
Moisture	7.00
Fixed Carbon	17.35
Volatile Mater	69.85
Ash	5.80
3. Lower calorific value (LHV)	
Corn stover (wet basis, 7% moisture)	14.970 (MJ/kg)

Table S2. Fast pyrolysis product composition (dry basis of biomass)

Compounds	Yield (%)
Non-condensable gas compounds	
Carbon dioxide	6.11
Carbon monoxide	5.77
Methane	0.11
Ethylene	0.12
Hydrogen	1.66
Propane	0.18
Ammonia	0.95
Sulfur dioxide	0.06
Hydrogen sulfide	0.09
Bio-oil compounds	
Formic acid	5.91
Acetic acid	3.05
Glycolaldehyde	4.13
Hydroxyacetone	3.91
Furfural	3.44
2(5H)-Furanone	1.81
Levoglucosan	6.51
Glucose	5.66
Phenol	3.86
Guaiacol	6.25
Xylenol	5.71
Eugenol	5.58
Water	13.33
Other compounds	
Char (including ash)	15.80

Table S3. Polyol product composition

Compounds	Composition (tonnes/d)
Ethylene glycol	1.259
Propylene glycol	1.553
Butanediol	0.354
Pentylene glycol	0.870
Cyclohexanediol	0.055
Total	4.091

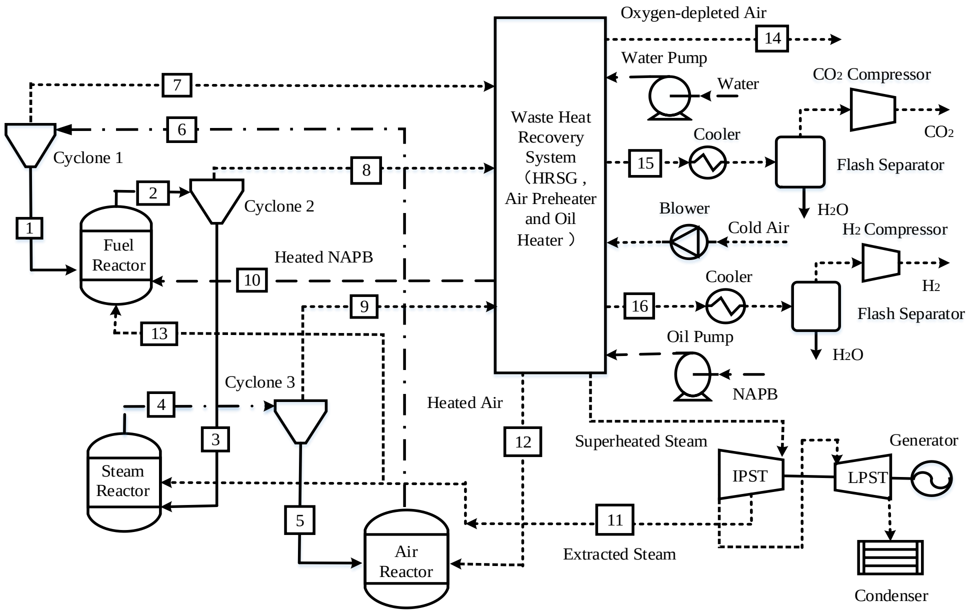

Figure S2. Process flow diagram of chemical looping hydrogen production system using non-aqueous phase bio-oil (NAPB) as fuel: (solid lines) solid streams; (dotted and dashed lines) gas-solid steams; (dashed lines) liquid streams; (dotted lines) gaseous streams.

Table S4. Key assumptions and self-sustaining operating conditions for the process simulation of chemical-looping hydrogen production

Item	Description or Value
Ambient condition	T = 25 ℃, P = 0.101 MPa
Reaction assumptions	all reactions reach equilibrium unless otherwise specified
Heat loss in the overall system	1% of the total thermal input
NAPB conversion in FR	100%
Fuel reactor	temperature, 850 ℃; pressure,0.101 MPa
Steam reactor	temperature, 750 ℃; pressure,0.101 MPa
Air reactor	temperature, 1030 ℃; pressure, 0.101 MPa
Convective heat exchangers	pressure drop , 2%; approach point ΔT,10 °C
Mechanical efficiency of all pressure changers	0.99
Isentropic efficiency of air blowers and pumps	0.83
CO_2 compressor specifications	4 stages with intercooler outlet temperature at 30 ℃; isentropic efficiency, 0.85; outlet pressure , 12 MPa; cooling water inlet temperature, 15 ℃; pressure loss in the heat exchanger, 3%;
H_2 compressor specifications	4 stages with intercooler outlet temperature at 30 ℃; isentropic efficiency, 0.85; outlet pressure, 6 MPa; cooling water inlet temperature, 15 ℃; pressure loss in the heat exchanger, 3%.
Air feed	10% excess (by mole)
Isentropic efficiency of steam turbines	0.87
Mechanical efficiency of couplers	0.99
Generator efficiency	0.92

Table S5. Process simulation results of self-sustaining operation mode of chemical-looping hydrogen production (LHV basis)

Item	Value
Operating temperature of air reactor(^{o}C)	1030
Feedstock carbon conversion rate in fuel reactor	100%
Solid circulating rate (kg/h)	9334.2
Iron oxide loading proportion (wt.)	83.6%
Mole ratio of fresh Fe_2O_3 in oxygen carrier to carbon in fuel	3.50
Solid conversion rate in fuel reactor	22.0%
Steam conversion rate in steam reactor	44.1%
Air flow rate in air reactor (kg/h)	1235.6
Steam flow rate in steam reactor (kg/h)	649.7
Total CO_2 production flow rate in fuel reactor (kg/h)	593.7
H_2 production flow rate (kg/h)	32.08
H_2 mole fraction in gases in steam reactor (dry basis)	100%
NO production flow rate in air reactor (kg/h)	0.169
NO_2 production flow rate in air reactor (kg/h)	0.0009
Fuel Reactor net heat duty Q_{FR} (MW)	-1.2E-06
Steam Reactor net heat duty Q_{SR} (MW)	-0.285
Air Reactor net heat duty Q_{AR} (MW)	-0.005
Total thermal efficiency (η_{tot})	58.0%
Hydrogen thermal efficiency (η_{H2})	57.9%
Net electricity efficiency (η_{e})	-0.12%
Net efficiency of CO_2 capture (η_{CO2}) (assumed conservatively)	90%

Table S6. Inventory data for biomass production (dry basis)

Item	Amount	Unit
Outputs of resources		
Harvested corn stover	1	kg
Inputs of resources		
Herbicide	0.093	g
Insecticide	0.034	g
N fertilizer	6.60	g
P_2O_5	2.05	g
K_2O	2.05	g
Electricity for field irrigation	0.004	kWh
Direct emission to air		
N_2O	0.082	g
NO	0.083	g

Table S7. Inventory data for biomass collection and transportation

Item	Amount	Unit
Outputs of resources		
Delivered corn stover (25 wt.% moisture)	33.5	tonnes
Input of resources		
Collected corn stover	33.5	tonnes
Diesel fuel for corn stover harvester	104.5	kg
Electricity for baling corn stover	217.8	kWh
Diesel fuel for corn stover loader	8.19	kg
Tractor 0.65 tonnes	66	tonne•km
Truck 8 tonnes	463	tonne•km

Table S8. Inventory data for biomass pre-treatment

Item	Amount	Unit
Outputs of resources		
Pre-treated corn stover (7 wt.% moisture)	26.9	tonnes/d
Inputs of resources		
Delivered corn stover (25wt.% moisture)	33.5	tonnes /d
Steam for drying biomass	2.71	tonnes/d
Electricity for chopping	570	kWh/d
Electricity for grinding	1345	kWh/d
Electricity for compressor	726	kWh/d
Emission to air		
Water steam	9.20	tonnes/d

Table S9. Inventory data for bio-oil production

Item	Amount	Unit
outputs		
Pyrolysis bio-oil	19.18	tonnes/d
Char	1.04	tonnes/d
Avoided products		
Mined raw coal	1.01	tonnes/d
Inputs of resources		
Air input in combustor	52.61	tonnes/d
Process water	220.95	tonnes/d
Solid heat carrier（SiO_2 : solids circulating rate）	124.39	tonnes/d
Pre-treated corn stover	26.90	tonnes/d
Electricity for pyrolysis	6823	kWh/d
Direct emission to air (from the combustor)		
N_2	40.550	tonnes/d
O_2	2.840	tonnes/d
CO (biogenic)	1-e6	tonnes/d

CO_2 (biogenic)	10.430	tonnes/d
SO_2	0.057	tonnes/d
NO	0.007	tonnes/d
NO_2	0.0001	tonnes/d
Water steam	4.255	tonnes/d
Solid waste to processing		
Ash	1.150	tonnes/d

Table S10. Inventory analysis for hydrogen and polyol production

Item	Amount	Unit
Outputs		
Polyol fuel	4.091	tonnes/d
Esters by-product	2.880	tonnes/d
Surplus hydrogen	0.576	tonnes/d
Inputs of resources		
Pyrolysis bio-oil (containing water)	19.18	tonnes/d
Consumed methanol	1.222	tonnes/d
Electricity for upgrading	1074	kWh/d
Ru/C catalyst (particle circulation rate)	0.261	tonnes/d
Pt/C catalyst (particle circulation rate)	0.261	tonnes/d
Air input in air reactor	29.653	tonnes/d
Fe_2O_3 power (particle circulation rate)	7.800	tonnes/d
Al_2O_3 power (particle circulation rate)	1.534	tonnes/d
Water working medium for CLHP	6.900	tonnes/d
Process water for CLHP	851	tonnes/d
Direct emission to air (from Air Reactor)		
N_2	22.360	tonnes/d
O_2	0.623	tonnes/d
CO_2	0.014	tonnes/d
NO	0.004	tonnes/d
NO_2	2.14e-5	tonnes/d
Water steam	0.016	tonnes/d
Waste to be treated		
Waste water	7.80	tonnes/d

Table S11. Inventory data for polyol transportation and distribution

Item	Amount	Unit
Outputs		
Delivered polyols	8	tonnes
Inputs		
Polyols	8	tonnes
Truck 8 tonnes for transportation	1200	tonne•km
Truck 8 tonnes for distribution	360	tonne•km

Table S12. Inventory data for polyol consumption

Item	Amount	Unit
Outputs		
Output energy	1	MJ
Inputs of resources		
Polyols	0.0451	kg
Direct emissions to air		
CO_2	0.0782	kg
CO	7.44e-05	kg
CH_4	1.30e-04	kg
HC	4.67e-06	kg