Production of furanics from sugarcane bagasse via the 5-chloromethylfurfural pathway: techno-economics and greenhouse gas assessment

Jerome Ramirez[a,b,d*], *Aban Sakheta*[a,b], *Lalehvash Moghaddam*[a,c], *Darryn Rackemann*[a,b], *Gabriel Fraga*[a,b]

[a] Centre for Agriculture and the Bioeconomy, Queensland University of Technology, Brisbane, QLD, 4000 Australia

[b] School of Mechanical, Medical, and Process Engineering, Faculty of Engineering, QUT, Brisbane, Australia

[c] School of Chemistry & Physics, Faculty of Science, Queensland University of Technology, Brisbane, Australia

[d] Australian Research Council Centre of Excellence in Synthetic Biology, QUT, Brisbane, Australia

Corresponding Author:

E-mail: j2.ramirez@qut.edu.au

Table S1. Bagasse composition (dry basis) for the model.

Component	Weight concentration
Glucan	43.0%
Xylan	17.0%
Arabinan	1.7%
Galactan	0.8%
Lignin	21.5%
Extractives	5.2%
Ash	8.2%
Acetate	2.6%

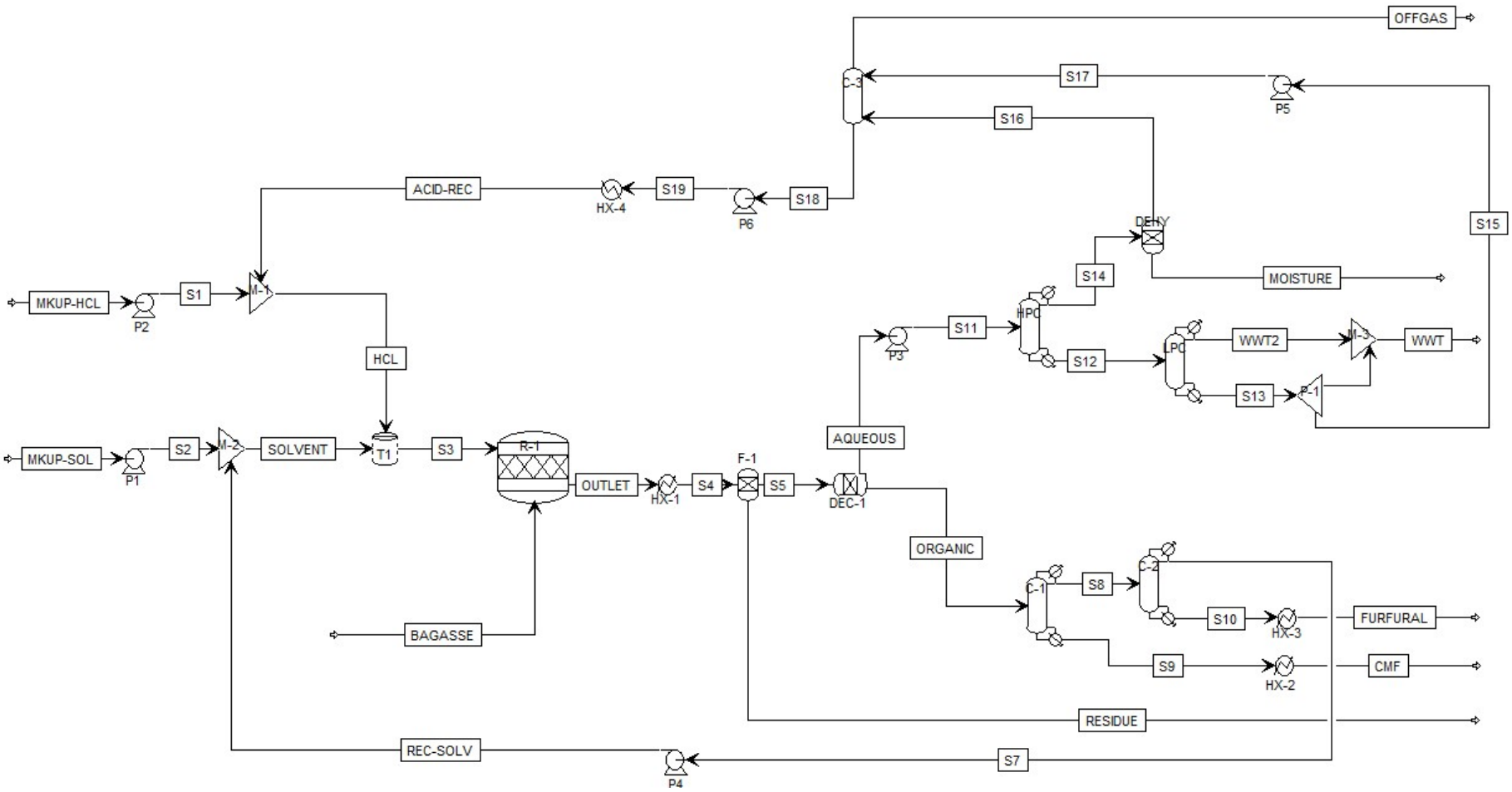

Figure S1. Process flow diagram for production of CMF from sugarcane bagasse.

Reactions (in series):

GLUCAN + WATER → GLUCOSE	(1)	100% conversion
XYLAN + WATER → XYLOSE	(2)	100% conversion
ARABINAN + WATER → ARABINOSE	(3)	100% conversion
GALACTAN + WATER → GALACTOSE	(4)	100% conversion
LIGNIN → LIGNIN SOLUBILISED	(5)	15% conversion
GLUCOSE + HCl → CMF + 4 H_2O	(6)	70% conversion
GLUCOSE → LEVACID + FORACID + WATER	(7)	10% conversion
2GLUCOSE → CHAR + WATER	(8)	100% conversion
ARABINOSE → FURFURAL + 3 H_2O	(9)	50% conversion
2ARABINOSE → FUROIN + 6H_2O	(10)	100% conversion
GALACTOSE + HCL → CMF + 4 H_2O	(11)	70% conversion
GALACTOSE → LEVACID + FORACID + H_2O	(12)	10% conversion
2GALACTOSE → CHAR + WATER	(13)	100% conversion
XYLOSE → FURFURAL + 3H_2O	(14)	50% conversion
2XYLOSE → FUROIN + 6 H_2O	(15)	100% conversion
ACETATE → ACETIC ACID	(16)	100% conversion
2EXTRACT → CHAR + H_2O	(17)	100% conversion
FORACID → H_2O + CO	(18)	100% conversion

*LEVACID = levulinic acid; FORACID = formic acid; CHAR = humins; FUROIN = humins

Table S2. Process stream table for production of CMF from sugarcane bagasse

	Units	ACID-REC	AQUEOUS	BAGASSE	CMF	FURFURAL	HCL	MKUP-HCL	MKUP-SOL	MOISTURE	OFFGAS	ORGANIC	OUTLET
Temperature	C	40.0	40.0	25.0	40.0	40.0	25.6	25.0	25.0	128.5	167.3	40.0	110.0
Pressure	bar	15.0	1.0	15.0	1.0	0.5	15.0	1.0	1.0	10.0	10.0	1.0	15.0
Mass Flows	kg/hr	38556.84	56816.12	30000.00	7283.35	1732.33	49832.49	49832.49	1282.89	791.39	6.55	107397.86	179497.55
Mass Fractions													
H2O		0.605	0.671	0.100	0.000	0.000	0.630	0.630	0.000	0.558	0.262	0.000	0.215
HCL		0.362	0.289	0.000	0.000	0.000	0.370	0.370	0.000	0.105	0.734	0.000	0.092
GLUCOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EXTRACT		0.000	0.000	0.038	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AACID		0.002	0.012	0.000	0.000	0.000	0.000	0.000	0.000	0.139	0.002	0.007	0.008
ACETATE		0.000	0.000	0.024	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLAN		0.000	0.000	0.155	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINAN		0.000	0.000	0.015	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GLUCAN		0.000	0.000	0.391	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTAN		0.000	0.000	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FURFURAL		0.002	0.002	0.000	0.000	0.996	0.000	0.000	0.000	0.002	0.001	0.016	0.010
FORACID		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LEVACID		0.002	0.002	0.000	0.023	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.001
CHAR		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.025
LIGNIN		0.000	0.000	0.195	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.028
LIGNSOL		0.020	0.015	0.000	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005
DCE		0.000	0.005	0.000	0.000	0.000	0.000	0.000	1.000	0.196	0.000	0.909	0.551
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ASH		0.000	0.000	0.075	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.013
5-CMF		0.007	0.005	0.000	0.971	0.004	0.000	0.000	0.000	0.000	0.000	0.066	0.042
FUROIN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010
Volume Flow	m^3/hr	32.66	49.63	61.25	5.27	1.52	42.11	42.12	1.03	94.08	0.81	87.31	192.68

	Units	REC-SOLV	RESIDUE	S1	S2	S3	S4	S5	S7	S8	S9	S10	S11
Temperature	C	63.9	40.0	25.6	26.1	38.1	40.0	40.0	62.8	84.1	257.1	137.4	40.3
Pressure	bar	15.0	1.0	15.0	15.0	15.0	1.0	1.0	0.5	1.0	1.0	0.5	10.0
Mass Flows	kg/hr	98382.18	15283.57	49832.49	1282.89	149497.55	179497.55	164213.98	98382.18	100114.51	7283.35	1732.33	56816.12
Mass Fractions													
H2O		0.000	0.025	0.630	0.000	0.210	0.215	0.232	0.000	0.000	0.000	0.000	0.671
HCL		0.000	0.011	0.370	0.000	0.123	0.092	0.100	0.000	0.000	0.000	0.000	0.289
GLUCOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EXTRACT		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AACID		0.007	0.001	0.000	0.000	0.005	0.008	0.009	0.007	0.007	0.000	0.000	0.012
ACETATE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GLUCAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FURFURAL		0.000	0.001	0.000	0.000	0.000	0.010	0.011	0.000	0.017	0.000	0.996	0.002
FORACID		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LEVACID		0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.000	0.023	0.000	0.002
CHAR		0.000	0.294	0.000	0.000	0.000	0.025	0.000	0.000	0.000	0.000	0.000	0.000
LIGNIN		0.000	0.325	0.000	0.000	0.000	0.028	0.000	0.000	0.000	0.000	0.000	0.000
LIGNSOL		0.000	0.001	0.000	0.000	0.000	0.005	0.005	0.000	0.000	0.006	0.000	0.015
DCE		0.992	0.065	0.000	1.000	0.662	0.551	0.596	0.992	0.975	0.000	0.000	0.005
CO		0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ASH		0.000	0.147	0.000	0.000	0.000	0.013	0.000	0.000	0.000	0.000	0.000	0.000
5-CMF		0.000	0.005	0.000	0.000	0.000	0.042	0.045	0.000	0.000	0.971	0.004	0.005
FUROIN		0.000	0.121	0.000	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000	0.000
Volume Flow	m^3/hr	82.85	172.39	42.11	1.03	123.44	255.58	136.91	82.73	86.67	6.47	1.68	49.62

	Units	S12	S13	S14	S15	S16	S17	S18	S19	SOLVENT	WWT	WWT1	WWT2
Temperature	C	185.6	108.3	128.5	108.3	128.5	108.5	117.2	117.4	63.5	49.3	108.3	40.0
Pressure	bar	10.0	1.0	10.0	1.0	10.0	10.0	10.0	15.0	15.0	1.0	1.0	1.0
Mass Flows	kg/hr	47815.98	32815.98	9000.00	30354.78	8208.61	30354.78	38556.84	38556.84	99665.05	17461.20	2461.20	15000.00
Mass Fractions													
H2O		0.788	0.768	0.049	0.768	0.000	0.768	0.605	0.605	0.000	0.821	0.768	0.830
HCL		0.169	0.190	0.921	0.190	1.000	0.190	0.362	0.362	0.000	0.134	0.190	0.125
GLUCOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLOSE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINOS		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EXTRACT		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AACID		0.012	0.002	0.012	0.002	0.000	0.002	0.002	0.002	0.007	0.030	0.002	0.035
ACETATE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
XYLAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ARABINAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GLUCAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GALACTAN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FURFURAL		0.002	0.003	0.000	0.003	0.000	0.003	0.002	0.002	0.000	0.002	0.003	0.001
FORACID		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LEVACID		0.002	0.003	0.000	0.003	0.000	0.003	0.002	0.002	0.000	0.000	0.003	0.000
CHAR		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIGNIN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIGNSOL		0.017	0.025	0.000	0.025	0.000	0.025	0.020	0.020	0.000	0.004	0.025	0.000
DCE		0.003	0.000	0.017	0.000	0.000	0.000	0.000	0.000	0.992	0.008	0.000	0.009
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ASH		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5-CMF		0.006	0.009	0.000	0.009	0.000	0.009	0.007	0.007	0.000	0.001	0.009	0.000
FUROIN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Volume Flow	m^3/hr	49.96	31.23	830.36	28.89	735.28	28.89	34.76	34.76	83.88	16.47	2.34	14.16

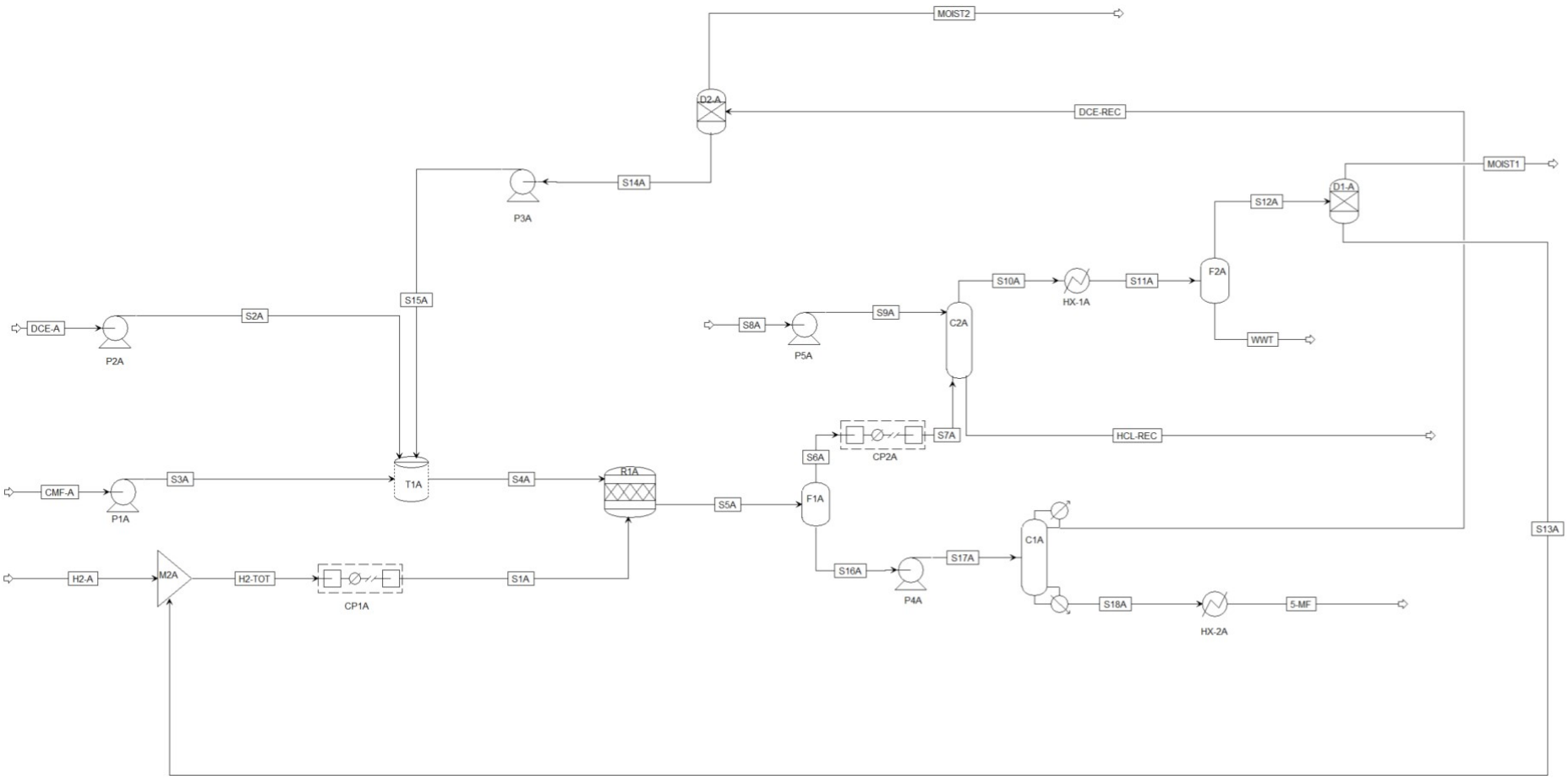

Figure S2. Process flow diagram for production of 5-MF from CMF.

Reaction:

$CMF + H_2 \rightarrow 5\text{-MF} + HCl$ (19) 100% conversion

Table S3. Process stream table for production of 5-MF from CMF

	Units	5-MF	CMF-A	DCE-A	DCE-REC	H2-A	H2-TOT	HCL-REC	MOIST1	MOIST2	S1A	S2A	S3A	S4A	S5A
Temperature	C	40.0	40.0	25.0	37.2	25.0	35.2	88.1	40.0	37.2	50.0	27.3	42.4	39.9	70.0
Pressure	bar	1.3	1.0	1.0	1.3	1.0	1.0	10.0	10.0	1.3	25.0	30.0	30.0	30.0	25.0
Mass Flows	kg/hr	5700.00	7283.35	193.04	35475.79	98.52	295.57	3949.08	10.52	343.68	295.57	193.04	7283.35	42608.50	42904.07
Mass Fractions															
H2O		0.000	0.000	0.000	0.000	0.000	0.000	0.630	0.829	0.000	0.000	0.000	0.000	0.000	0.000
HCL		0.000	0.000	0.000	0.010	0.000	0.000	0.348	0.017	1.000	0.000	0.000	0.000	0.000	0.042
LEVACID		0.038	0.030	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.005	0.005
DCE		0.018	0.000	1.000	0.990	0.000	0.000	0.022	0.154	0.000	0.000	1.000	0.000	0.829	0.823
5-CMF		0.000	0.970	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.970	0.166	0.000
H2		0.000	0.000	0.000	0.000	1.000	1.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.005
5-MF		0.944	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.125
Volume Flow	m³/hr	5.22	5.27	0.15	28.93	1212.23	3761.45	3.48	0.01	185.96	159.83	0.16	5.28	34.26	43.63

	Units	S6A	S7A	S8A	S9A	S10A	S11A	S12A	S13A	S14A	S15A	S16A	S17A	S18A	WWT
Temperature	C	-20.0	40.0	25.0	25.1	121.6	40.0	40.0	40.0	37.2	39.5	-20.0	-19.9	191.8	40.0
Pressure	bar	1.0	10.0	1.0	10.0	10.0	10.0	10.0	10.0	1.3	30.0	1.0	2.0	1.3	10.0
Mass Flows	kg/hr	1728.28	1728.28	2800.00	2800.00	579.20	579.20	207.56	197.05	35132.11	35132.11	41175.79	41175.79	5700.00	371.63
Mass Fractions															
H2O		0.000	0.000	1.000	1.000	0.539	0.539	0.042	0.000	0.000	0.000	0.000	0.000	0.000	0.816
HCL		0.832	0.832	0.000	0.000	0.113	0.113	0.001	0.000	0.000	0.000	0.008	0.008	0.000	0.175
LEVACID		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.005	0.038	0.000
DCE		0.054	0.054	0.000	0.000	0.008	0.008	0.008	0.000	1.000	1.000	0.856	0.856	0.018	0.009
5-CMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2		0.114	0.114	0.000	0.000	0.340	0.340	0.949	1.000	0.000	0.000	0.000	0.000	0.000	0.000
5-MF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.131	0.131	0.944	0.000
Volume Flow	m³/hr	2905.80	359.34	2.81	2.81	384.44	257.62	257.28	255.98	28.59	28.67	32.12	32.12	6.10	0.34

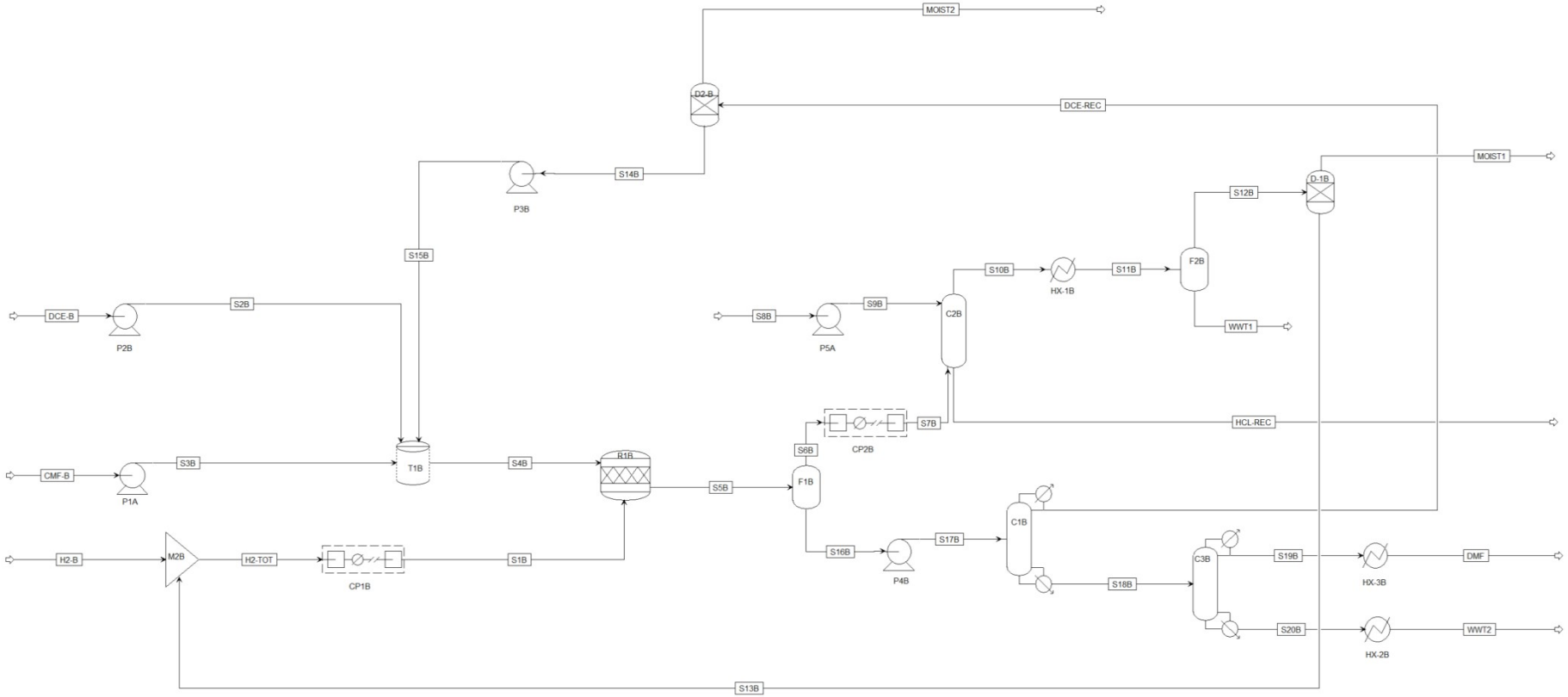

Figure S3. Process flow diagram for production of DMF from CMF.

Reactions (in series):

$CMF + 3H_2 \rightarrow DMF + HCl + H_2O$ (20) 93% conversion

$CMF + 2H_2 \rightarrow HCl + MFA$ (21) 100% conversion

*MFA = 5-methylfurfuryl alcohol

Table S4. Process stream table for production of DMF from CMF

	Units	CMF-B	DCE-B	DCE-REC	DMF	H2-B	H2-TOT	HCL-REC	MOIST1	MOIST2	S1B	S2B	S3B	S4B	S5B	S6B
Temperature	C	40.0	25.0	89.1	40.0	25.0	32.8	76.7	40.0	89.1	50.0	27.3	42.4	83.7	50.0	-20.0
Pressure	bar	1.0	1.0	2.5	1.0	1.0	1.0	10.0	10.0	2.5	30.0	30.0	30.0	30.0	30.0	1.0
Mass Flows	kg/hr	7283.35	130.32	36074.17	3800.00	288.67	591.12	3949.10	17.03	880.21	591.12	130.32	7283.35	42607.63	43198.72	1924.55
Mass Fractions																
H2O		0.000	0.000	0.000	0.025	0.000	0.000	0.620	0.549	0.006	0.000	0.000	0.000	0.000	0.019	0.000
HCL		0.000	0.000	0.008	0.000	0.000	0.000	0.351	0.242	0.323	0.000	0.000	0.000	0.000	0.041	0.778
LEVACID		0.030	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.005	0.005	0.000
DCE		0.000	1.000	0.976	0.004	0.000	0.000	0.028	0.205	0.000	0.000	1.000	0.000	0.829	0.818	0.061
5-CMF		0.970	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.970	0.166	0.000	0.000
FUROIN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMF		0.000	0.000	0.016	0.971	0.000	0.000	0.002	0.004	0.671	0.000	0.000	0.000	0.000	0.101	0.004
MFA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.000
H2		0.000	0.000	0.000	0.000	1.000	1.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.007	0.157
Volume Flow	m³/hr	5.27	0.10	31.68	4.30	3551.84	7464.81	3.44	0.01	140.60	267.14	0.10	5.28	36.03	47.02	4048.85

	Units	S7B	S8B	S9B	S10B	S11B	S12B	S13B	S14B	S15B	S16B	S17B	S18B	S19B	S20B	WWT1	WWT2
Temperature	C	40.00	25.00	25.09	115.18	40.00	40.00	40.00	89.14	91.36	-20.00	-19.70	128.96	94.05	102.83	40.00	40.00
Pressure	bar	10.00	1.00	10.00	10.00	10.00	10.00	10.00	2.50	30.00	1.00	5.00	2.50	1.00	1.00	10.00	1.00
Mass Flows	kg/hr	1924.55	2800.00	2800.00	775.46	775.46	319.49	302.46	35193.96	35193.96	41274.17	41274.17	5200.00	3800.00	1400.01	455.97	1400.01
Mass Fractions																	
H2O		0.000	1.000	1.000	0.454	0.454	0.029	0.000	0.000	0.000	0.020	0.020	0.156	0.025	0.513	0.751	0.513
HCL		0.778	0.000	0.000	0.146	0.146	0.013	0.000	0.000	0.000	0.007	0.007	0.000	0.000	0.000	0.240	0.000
LEVACID		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.005	0.042	0.000	0.156	0.000	0.156
DCE		0.061	0.000	0.000	0.010	0.010	0.011	0.000	1.000	1.000	0.853	0.853	0.003	0.004	0.000	0.009	0.000
5-CMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FUROIN		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMF		0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.106	0.106	0.725	0.971	0.057	0.000	0.057
MFA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.009	0.074	0.000	0.274	0.000	0.274
H2		0.157	0.000	0.000	0.390	0.390	0.947	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Volume Flow	m³/hr	501.64	2.81	2.81	559.25	395.05	394.64	392.92	30.64	30.73	33.04	33.05	6.24	4.61	1.35	0.41	1.29

Table S5. GHG emissions of CMF produced from sugarcane bagasse

Inputs	Usage	Units per kg CMF	Assumptions	Value	Unit	GHG Emissions ($kgCO_2e$/kg CMF)
Hydrochloric acid transportation to Australia	14.2	tkm	Transoceanic tanker (from Kolkata port to Mackay port)	0.006	$kgCO_2e$/tkm	0.135
Dichloroethane transportation to Australia	1.12	tkm	Transoceanic tanker (from Osaka port to Mackay port)	0.006	$kgCO_2e$/tkm	0.011
Chemicals transportation to plant	0.06	tkm	Transport, truck, diesel powered (10 km from Mackay)	0.103	$kgCO_2e$/tkm	0.008
Bagasse transportation from other mills	0.034	tkm	Transport, truck, diesel powered (25 km)	0.103	$kgCO_2e$/tkm	0.007
Bagasse	4.12	kg	From sugar production	0.012	$kgCO_2e$/kg	0.047
Hydrochloric acid	1.55	kg	World market for HCl	0.878	$kgCO_2e$/kg	1.677
Dichloroethane	0.18	kg	World market for DCE	1.45	$kgCO_2e$/kg	0.256
Heat	43.1	MJ	Treatment of bagasse from sugarcane by combustion in heat and power cogeneration.	0.001	$kgCO_2e$/MJ	0.054
Electricity	0.015	kWh	Electricity from bagasse at mill	0.133	$kgCO_2e$/kWh	0.002
Liquid waste	0.002	m^3	Unspecified wastewater treatment	0.16	$kgCO_2e/m^3$	0.0003
Displacement of furfural	0.238	kg	Production from corncobs	-2.34	kgCO2e/kg	-0.558

Table S6. GHG emissions of 5-MF produced from sugarcane bagasse via CMF

Inputs	Usage	Units per kg 5MF	Assumptions	Value	Unit	GHG Emissions ($kgCO_2e$/kg CMF)
Hydrochloric acid transportation to Australia	11.76	tkm	Transoceanic tanker (from Kolkata port to Mackay port)	0.006	$kgCO_2e$/tkm	0.071
Dichloroethane transportation to Australia	1.65	tkm	Transoceanic tanker (from Osaka port to Mackay port)	0.006	$kgCO_2e$/tkm	0.001
Chemicals transportation to plant	0.02	tkm	Transport, truck, diesel powered (10 km from Mackay)	0.103	$kgCO_2e$/tkm	0.002
Bagasse transportation from other mills	0.034	tkm	Transport, truck, diesel powered (25 km)	0.103	$kgCO_2e$/tkm	0.007
Bagasse	5.26	kg	From sugar production	0.012	$kgCO_2e$/kg	0.061
Hydrochloric acid	1.29	kg	World market for HCl	0.878	$kgCO_2e$/kg	1.129
Dichloroethane	0.26	kg	World market for DCE	1.45	$kgCO_2e$/kg	0.377
Water	0.49	kg	Deionised water	0.0004	$kgCO_2e$/kg	0.0002
Hydrogen	0.017	kg	World market for hydrogen	10.3	$kgCO_2e$/kg	0.176
Heat	63.2	MJ	Treatment of bagasse from sugarcane by combustion in heat and power cogeneration.	0.001	$kgCO_2e/m^3$	0.080
Electricity	0.25	kWh	Electricity from bagasse at mill	0.133	$kgCO_2e$/kWh	0.033
Liquid waste	0.003	m^3	Unspecified wastewater treatment	0.16	$kgCO_2e/m^3$	0.0003
Displacement of furfural	0.30	kg	Production from corncobs	-2.34	kgCO2e/kg	-0.713

Table S7. GHG emissions of DMF produced from sugarcane bagasse via CMF

Inputs	Usage	Units per kg DMF	Assumptions	Value	Unit	GHG Emissions ($kgCO_2e$/kg DMF)
Hydrochloric acid transportation to Australia	17.63	tkm	Transoceanic tanker (from Kolkata port to Mackay port)	0.006	$kgCO_2e$/tkm	0.106
Dichloroethane transportation to Australia	2.36	tkm	Transoceanic tanker (from Osaka port to Mackay port)	0.006	$kgCO_2e$/tkm	0.014
Chemicals transportation to plant	0.01	tkm	Transport, truck, diesel powered (10 km from Mackay)	0.103	$kgCO_2e$/tkm	0.001
Bagasse transportation from other mills	0.034	tkm	Transport, truck, diesel powered (25 km)	0.103	$kgCO_2e$/tkm	0.007
Bagasse	7.89	kg	From sugar production	0.012	$kgCO_2e$/kg	0.091
Hydrochloric acid	1.93	kg	World market for HCl	0.878	$kgCO_2e$/kg	1.694
Dichloroethane	0.37	kg	World market for DCE	1.45	$kgCO_2e$/kg	0.537
Water	1.37	kg	Deionised water	0.0004	$kgCO_2e$/kg	0.0005
Hydrogen	0.08	kg	World market for hydrogen	10.3	$kgCO_2e$/kg	0.816
Heat	128	MJ	Treatment of bagasse from sugarcane by combustion in heat and power cogeneration.	0.001	$kgCO_2e$/MJ	0.160
Electricity	0.64	kWh	Electricity from bagasse at mill	0.133	$kgCO_2e$/kWh	0.085
Liquid waste	0.005	m^3	Unspecified wastewater treatment	0.16	$kgCO_2e/m^3$	0.001
Displacement of furfural	0.46	kg	Production from corncobs	-2.34	kgCO2e/kg	-1.070

Table S8. LCI data used for the emission factors from Tables S4-S6.

Item	Selected process for LCI	Database
Sea freight shipping	Transport, freight, sea, container ship GLO, market for transport, freight, sea, container ship, Cut-off, U	AusLCI
Road transport	Transport, truck, 16 to 28t, fleet average/AU U	AusLCI
Electricity	electricity from bagasse, at mill AU, U	AusLCI
Heating	Heat, district or industrial, other than natural gas RoW, treatment of bagasse, from sugarcane, in heat and power co-generation unit, 6400kW thermal, Cut-off, U	AusLCI
Cooling	Cooling energy RoW, cooling energy, from natural gas, at cogen unit with absorption chiller 100kW, Cut-off, U	AusLCI
Hydrogen	Hydrogen, gaseous, low pressure, RoW, hydrogen production, steam methane reforming, Cut-off, U	AusLCI
Hydrochloric acid	Hydrochloric acid, without water, in 30% solution state, RoW, market for hydrochloric acid, without water, in 30% solution state, Cut-off, U	AusLCI
Dichloroethane	Ethylene dichloride, RoW, market for ethylene dichloride, Cut-off, U	AusLCI
Water	Water, deionised, RoW, water production, deionised, Cut-off, U	AusLCI
Liquid waste incineration	Wastewater, average, RoW, market for wastewater, average, Cut-off, U	AusLCI
Displaced products:		
Furfural	Production of furfural from corncobs described in Fraga, et al. (Fraga et al., 2024)	

Reference

Fraga, G., Ramirez, J., Renouf, M., Batalha, N., 2024. Conceptual Process Design, Techno-Economics, and Greenhouse Gas Analysis of Furfuryl Alcohol Production via Transfer Hydrogenation. Acs Sustainable Chemistry & Engineering 12, 10604-10614.