Supplementary Information for

Sustainable production of 5-hydroxymethyl furfural from glucose for process integration with high fructose corn syrup infrastructure

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Tables and Figures

Table S1. Material balance information for selected streams based on the flowsheet in Figure 6.

Component	Units	1	3	4	5	6	8	9
Mass flow	$kg \cdot h^{-1}$	2,000	1,355	52,270	52,290	51,939	48,256	57,346
Temperature	^oC	25	25	65	120	120	30.1	30.1
Pressure	bar	1	1	3	10	10	1	1
Glucose	$kg \cdot h^{-1}$	2,000	0	1,130	961	951	0	951
Fructose	$kg \cdot h^{-1}$	0	0	1,967	216	214	31	183
HMF	$kg \cdot h^{-1}$	0	0	35	1,042	1042	1010	37
Acetone	$kg \cdot h^{-1}$	0	22	34,475	34,475	34,475	36,966	40,986
H_2O	$kg \cdot h^{-1}$	0	1,333	10,960	11,431	11,431	10,249	11,363
Humins	$kg \cdot h^{-1}$	0	0	0	281	0	0	0
BP	$kg \cdot h^{-1}$	0	0	3,703	3,864	3,826	0	3,826

Component	Units	10	11	12	15	17	19
Mass flow	$kg \cdot h^{-1}$	47,208	1048.5	45,413	9,175	8,245	744
Temperature	^oC	45	53.7	58	30.1	30	90
Pressure	bar	1.5	1.5	1	1	1	1
Glucose	$kg \cdot h^{-1}$	0	0	0	152	0	122
Fructose	$kg \cdot h^{-1}$	0	31.5	0	29	0	23
HMF	$kg \cdot h^{-1}$	4	1005.7	4	6	0	4
Acetone	$kg \cdot h^{-1}$	36,966	0.5	36,947	6,558	6,528	25
H_2O	$kg \cdot h^{-1}$	10,238	10.8	8,462	1,818	1,718	80
Humins	$kg \cdot h^{-1}$	0	0	0	0	0	0
BP	$kg \cdot h^{-1}$	0	0	0	612	0	490

Table S2. Installed costs and other relevant parameters for the main equipment.

Equipment	C_0($)	S_0	Units	Scaling basis	Base-year	β	Reference
R-1	406,000	113.6	m^3	Feed	2009	0.7	NREL[1]
R-2	406,000	113.6	m^3	Feed	2009	0.7	NREL[1]
S-1	288,000	55,927.0	$kg{\cdot}h^{-1}$	Feed	2017	0.6	Aspen Plus
S-2[a]	2,935,000	634.2	$kg{\cdot}h^{-1}$	Main product	1998	0.6	NREL[2]
S-3[b]	1,881,627	48,256.1	$kg{\cdot}h^{-1}$	Feed	2017	-	Aspen Plus
S-4	199,000	1,795.4	$kg{\cdot}h^{-1}$	Adsorbed water	2017	0.6	Aspen Plus
S-5[b]	635,500	9,175.4	$kg{\cdot}h^{-1}$	Feed	2017	-	Aspen Plus

[a] Includes the cost of adsorbent.

[b] Includes the cost of pumps, heaters, condensers, and flash columns.

Table S3. Summary of capital costs of a plant producing 8.74 kton/yr HMF.

Cost components		Total cost (MM$)
Inside-battery-limits (ISBL) equipment costs		10.13
Outside-battery-limits (OSBL) equipment costs	40.0% of ISBL	4.05
Warehouse	4.0% of ISBL	0.41
Site development	9.0% of ISBL	0.91
Additional piping	4.5% of ISBL	0.46
Total direct costs (TDC)		**15.96**
Prorateable expenses	10.0% of TDC	1.59
Field expenses	10.0% of TDC	1.59
Home office and construction fee	20.0% of TDC	3.19
Project contingency	40.0% of TDC	6.38
Other costs (Start-up, Permits, etc.)	10.0% of TDC	1.59
Total indirect costs		**14.36**
Fixed capital investment (FCI)		**30.32**
Land and working capital	5.0% of FCI	1.52
Total capital investment (TCI)		**31.84**

Table S4. Summary of operating costs for a 8.74 kton/yr HMF plant.

Raw material	Total cost (MM$/year)
Glucose	4.100
Acetone	0.150
Amberlyst-15 catalyst	0.043
Water	0.003
Activated carbon	0.0003
Molecular sieve adsorbent	0.020
Enzyme	0.043
Steam	1.420
Cooling water	0.100
Refrigerant	1.050
Electricity	0.010
Wastewater treatment	0.010
Disposal of ash	0.080
Total variable operating costs	7.039
Total fixed operating costs[a]	1.880
Total operating costs	**8.919**

[a] Fixed operating cost comprises of labor costs, annual maintenance, and property insurance, which are estimated as 4.5% of FCI, 3% of ISBL, and 0.7% of FCI.

Table S5. Economic parameters and assumptions.

Glucose price ($/ton) [a]	236
Acetone price ($/ton) [b]	800
Amberlyst-15 catalyst ($/kg) [a,b]	21
Activated carbon ($/kg) [a,b]	1.44
Molecular sieve adsorbent ($/kg) [b,c]	3.46
Enzyme ($/kg) [d,e]	50
Water ($/ton) [a]	0.3
Low pressure steam ($/kJ) [a]	3.26e-06
Cooling water ($/kJ) [a]	2.12e-07
-25^{o} C Refrigerant ($/kJ) [a]	7.89e-06
Electricity price ($/kWh) [a]	0.0572
Wastewater treatment cost ($/ton) [a]	0.57
Ash disposal ($/ton) [a]	35.39
Plant operating hours per year [a]	7884
Plant life (year) [a]	30
Internal rate of return (%) [a]	10
Plant depreciation (year) [a]	7
Loan terms [a]	10-year loan at 8% APR
Construction time (year) [a]	3
First 12 months' expenditure [a]	8
Next 12 months' expenditure [a]	60
Last 12 months' expenditure [a]	32
Federal tax rate (%) [a]	21
Financing (% of equity) [a]	40
Start-up time (month) [a]	6
Revenue during start-up (%) [a]	50
Variable operating costs during start-up (%) [a]	75
Fixed operating costs during start-up (%) [a]	100

[a] Taken from Motagamwala et al.[3]

[b] Refurbished after every 3 months at 20% of the initial cost.

[c] Taken from Urbaniec and Grabarczyk.[4]

[d] Refurbished after every 1.5 years at the initial cost.[5]

[e] Price of glucose-isomerase taken from Alibaba.[6]

Table S6. Relevant parameters for the analysis of integrated HFCS/HMF process.

Corn price ($/ton)	130[7]
Germ price ($/ton)	254[8]
Corn gluten feed price ($/ton)	95.2[7]
Corn gluten meal price ($/ton)	435.4[7]
Starch price ($/ton)	127[7]
HFCS-42 price ($/ton)	700[7]
HMF price ($/ton)	1500
Germ flow rate (kg/hr)	3393.5
Corn gluten feed flow rate (kg/hr)	8952.6
Corn gluten meal flow rate (kg/hr)	2673.9
Starch flow rate (kg/hr)	13100
Glucose flow rate from starch hydrolysis section (kg/hr)	18410
Percentage depreciation (% of TCI)	8

Table S7. TCI for a standalone HMF plant, greenfield and brownfield HFCS/HMF plants.

HMF production (kton/yr)	TCI for standalone HMF plant (MM$)	TCI for greenfield HFCS/HMF plant (MM$)	TCI for brownfield HFCS/HMF plant (MM$)
3.5	18.4	208.4	16.2
9.2	32.8	222.5	28.9
17.5	48.3	237.4	42.5

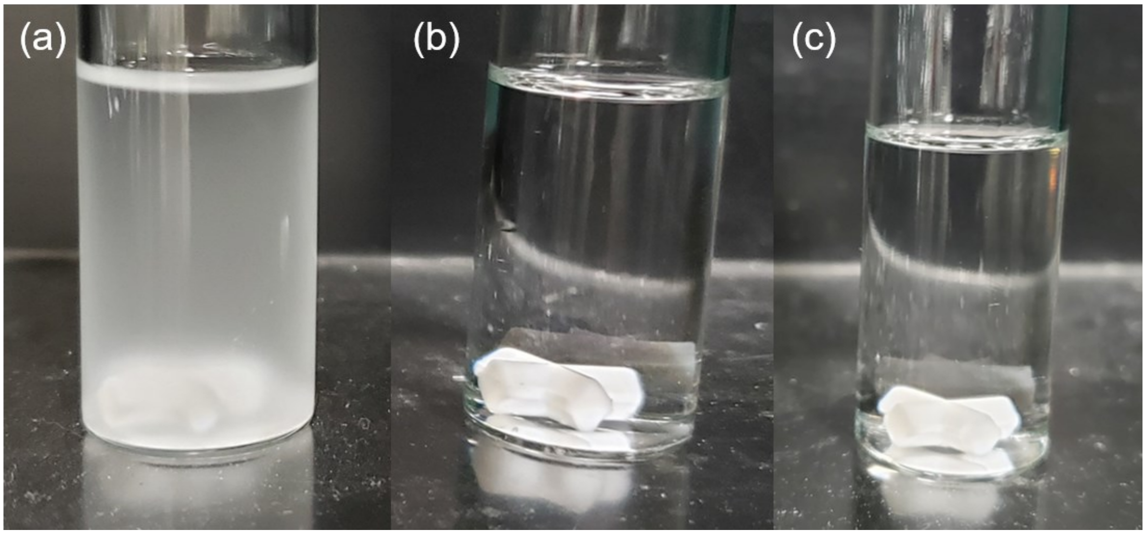

Figure S1. Image of (a) 5.7 wt% glucose (bi-phase), (b) 5.4 wt% glucose (mono-phase), and (c) 9.4 wt% fructose (mono-phase) in acetone/water (80/20, v/v) solvent. (The glucose and fructose solutions were kept at 65^{o}C for overnight and the images were taken before the temperature quenched to room temperature.

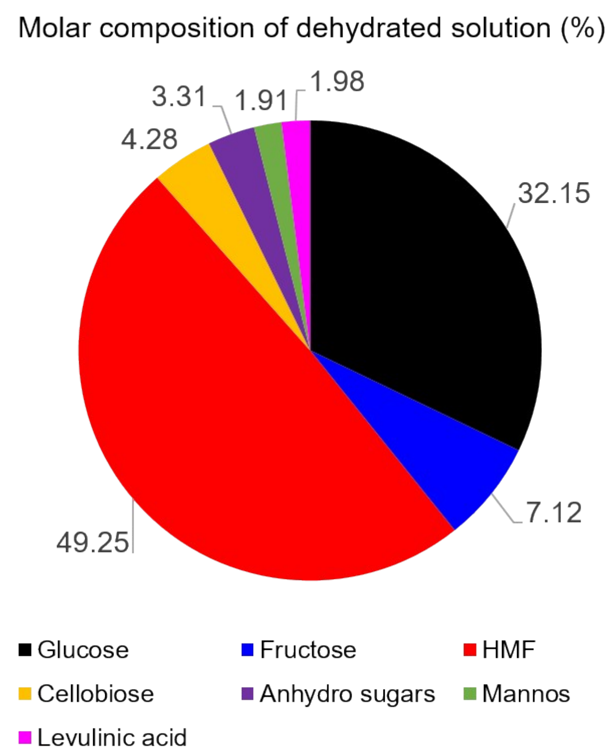

Figure S2. Molar composition (%) of the chemicals in the dehydrated solution.

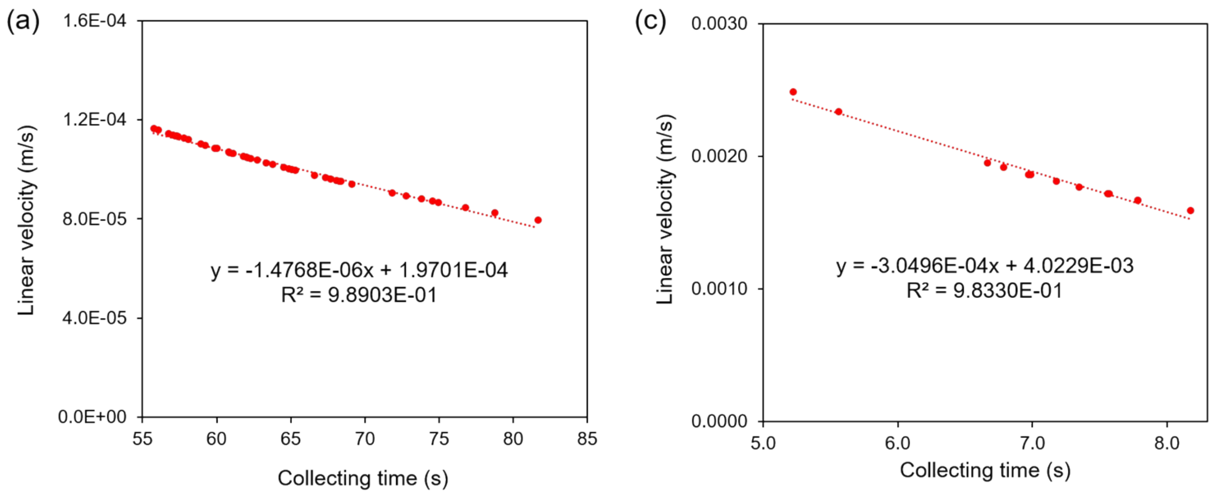

Figure S3. (a) Linear velocity (m·s^{-1}) of the loaded sample (mixture of glucose, fructose, and HMF) during the chromatography separation of HMF and sugar monomers, (b) Linear velocity (m·s^{-1}) of desorbent (acetone/water (80/20, v/v) solvent) during the collection of sugar monomers from the column.

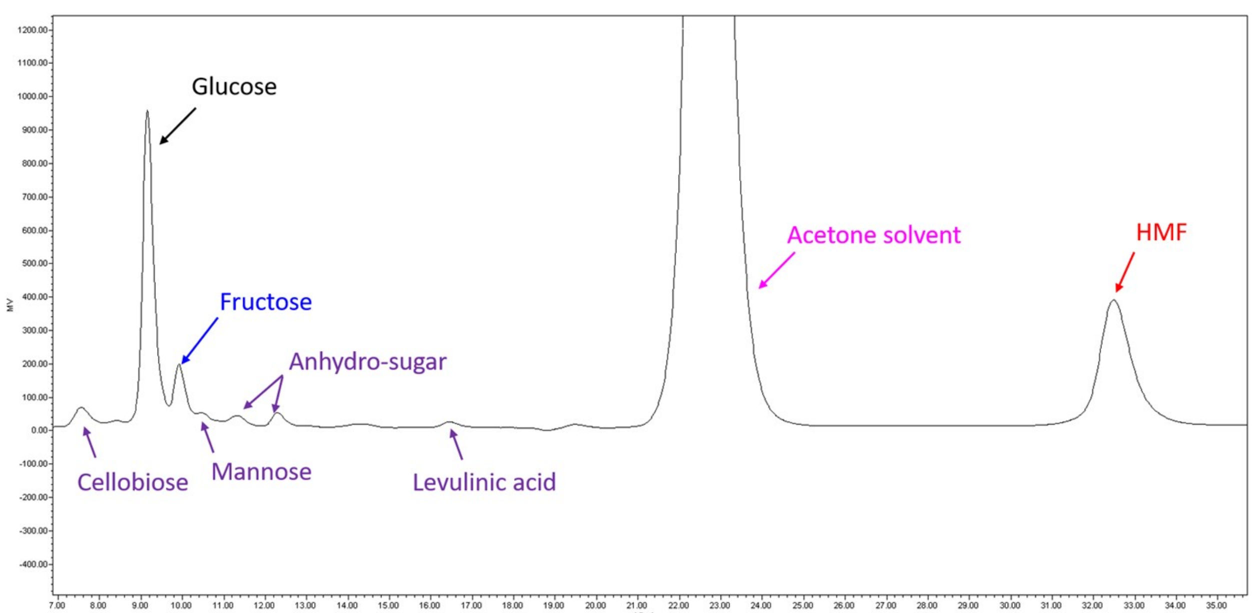

Figure S4. Retention time and chemical peaks on HPLC analysis of the dehydrated solution (Figure 2).

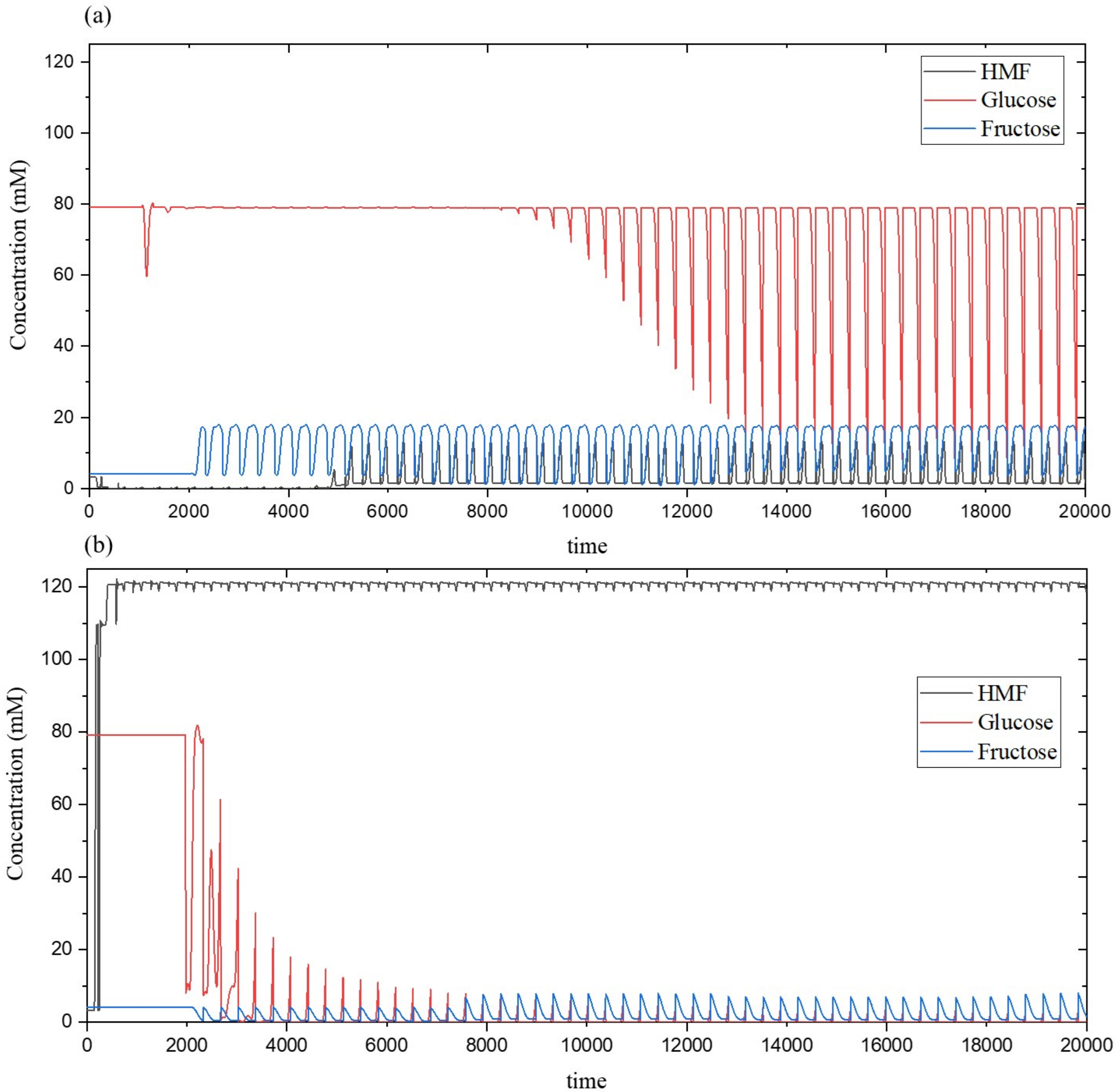

Figure S5. Concentration profiles of the components in the (a) extract and (b) raffinate streams. A four-zone SMB containing five columns in each zone is simulated with feed, desorbent, extract, and recycle flow rates set to 1.97 l/min, 2.22 l/min, 2.27 l/min, and 0.28 l/min, respectively. The port switching interval, column height, column diameter, inter-particle voidage, intra-particle voidage, and adsorbent particle radius are set to 350 min, 138.4 cm, 39 cm, 0.3 m^3 void/m^3 bed, 0.21 m^3 void/m^3 bead, 92.5 micron, respectively. Initially, none of the components are present in the columns. The purity and recovery of the components are calculated once cyclic steady state is achieved.

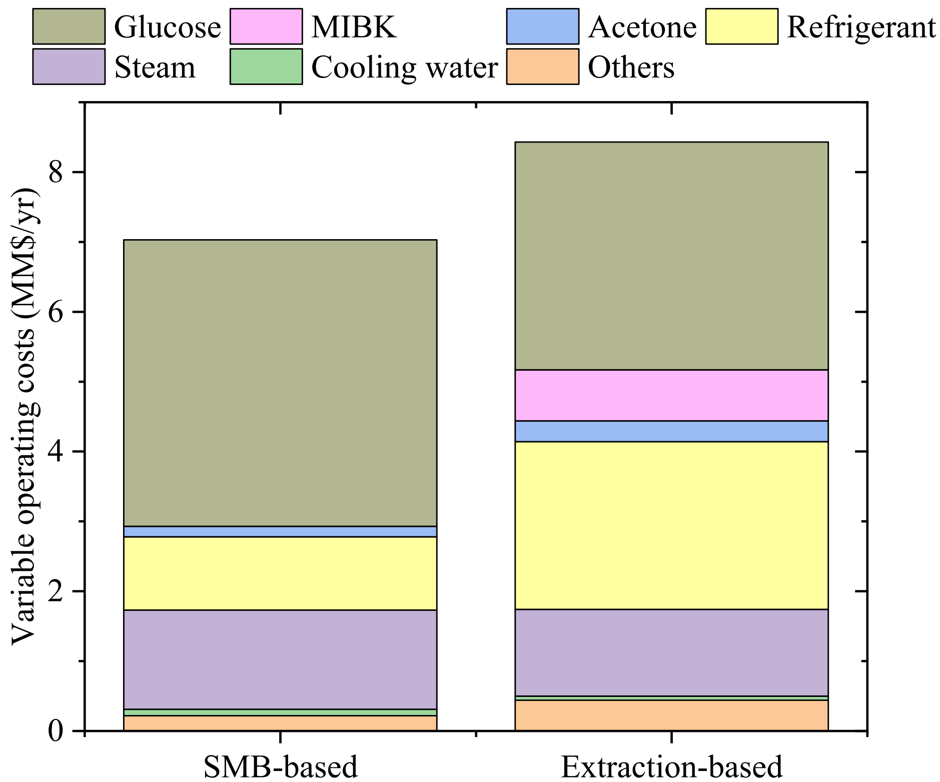

Figure S6. Comparison of variable operating costs of the proposed SMB-based and extraction-based approaches.

References

1 D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton and D. Dudgeon, *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover, NREL/TP-5100-47764*, 2011.

2 R. J. Wooley, D. Rice, F. Posey-Eddy, Z. Ma and N. H.-L. Wang, *Continuous Countercurrent Chromatographic Separator for the Purification of Sugars from Biomass Hydrolysate, NREL/TP-580-23907*, 1997.

3 A. H. Motagamwala, K. Huang, C. T. Maravelias and J. A. Dumesic, *Energy Environ. Sci.*, 2019, **12**, 2212–2222.

4 K. Urbaniec and R. Grabarczyk, *J. Clean. Prod.*, 2014, **65**, 324–329.

5 E. Papadakis, S. Pedersen, A. K. Tula, M. Fedorova, J. M. Woodley and R. Gani, *Comput. Chem. Eng.*, 2017, **98**, 128–142.

6 Alibaba, Glucose isomerase price, https://www.alibaba.com/product-detail/Factory-Supply-Hot-Sale-Food-Additives_62219234715.html?spm=a2700.galleryofferlist.0.0.4d635475Gw8xMF, (accessed 2 June 2020).

7 T. Capehart, O. Liefert, D. Olson and S. Proper, *USDA ERS Feed Outlook |Corn Crop Grows on Yield*, 2019.

8 Zauba, Import data of corn germ, https://www.zauba.com/import-corn+germ-hs-code.html, (accessed 22 June 2020).