

Supporting Information

Converting Food Waste into High-value Medium Chain Fatty Acids and Long Chain Alcohols via Chain Elongation with Internally Produced Electron Donor

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Table S1 FW composition and values in different countries.

Countries or regions	FW composition	FW volume	GNI	The proportion of bioresource recovery via AD
Denmark	Carbohydrate mainly, including wheat, sugar, pasta, rice, etc. ¹	2.2 million tons. ²	65,520 US\$	10%
Canada	Carbohydrate mainly.	<ul style="list-style-type: none"> • 12.6 million tons of FW was directly sent to landfill for final disposal. • 5.8 million tons of organics FW are diverted to alternative treatment. 	<ul style="list-style-type: none"> • The monetary value of avoidable food loss and waste alone was US\$ 27 billion in 2010.³ • Such value is slightly lower than the value of all Canadian agricultural and agri-food exports in 2007.³ 	-
US	Carbohydrate mainly. Lipid and other carbon containing materials are also the key composition of FW.	28.8 million tons. ⁴	<ul style="list-style-type: none"> • 53,670 US\$ • Accounting for \$75 billion of the American economy annually in total.⁵ 	<3% ⁴
China	Carbohydrate mainly. Rice and pasta contribute to up to 70.2% of FW. ⁶	82.8 million tons. ⁷	6,560 US\$	7% ⁶
South Korea	Carbohydrate mainly.	4.2-5.5 million tons. ⁸	25,920 US\$ Only 10% of the FW was treated via AD in 2008.	10% ⁹

AD: anaerobic digestion; GNI: Gross National Index.

1 Electron transfer efficiency of the various fermentative systems

The electron transfer efficiency indicated how many electrons from food waste (FW) were transferred to the fermentative products. The electron transfer efficiency in the fermentation system with or without yeast inoculation was calculated using **Eq. 1**. All the involved compounds and their electrons are: 12/ethanol, 18/propanol, 24/butanol, 30/pentanol, 36/hexanol, 2/H₂, 8/acetate, 14/propionate, 20/butyrate, 26/valerate, 32/caproate, 38/heptylate, 44/caprylate.^{10, 11} **Table S2** demonstrated the electron transfer efficiency in various fermentative systems.

$$\text{Electron efficiency \%} = \frac{\text{Products (mmol } e^{-})}{\text{FW (mmol } e^{-})} \quad 1)$$

Table S2 Electron transfer efficiency in various fermentative systems.

Fermentation system	Electron efficiency (%)
Control	18.08
1Y	19.32
1.5Y	41.04
3Y	51.46
4Y	61.18

Table S3 The Standard free Gibbs energy ($\Delta_f G^0_{i,Ts}$) of possible substances involved in MCFAs and butanol production from FW-contained fermentation with in-situ ethanol provision. The values were adapted or calculated according to Kleerebezem and Van Loosdrecht (2010).¹²

Name	$\Delta_f G^0_{i,Ts}$ (KJ/mol)
H ₂ O	-237.2
ethanol	-181.8
n-butanol	-171.8
acetate	-369.4
propionate	-367.3
n-butyrate	-358.7
n-valerate	-350.2
n-caproate	-341.8
n-heptanoate	-333.2
n-caprylate	-324.6
H ⁺	0
H ₂	0
CO ₂	-394.4
Glucose	-910.56

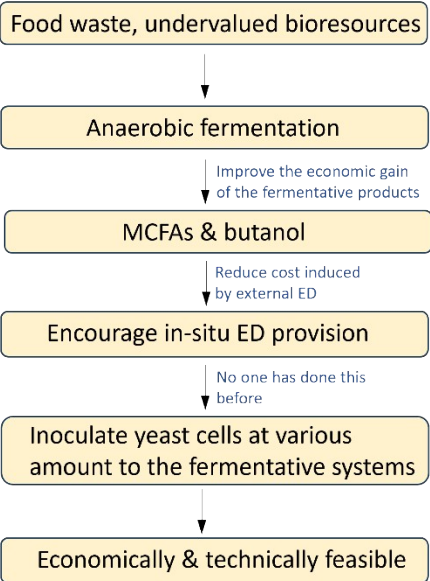
Table S4 Thermodynamic information for the chain elongation reactions, butanol production and in-situ ethanol biosynthesis (Ts: temperature of standard condition)

Equation	ΔG^0_{Ts} (KJ mol ⁻¹)
Chain elongation	
Re.1 $6\text{CH}_3\text{CH}_2\text{OH} + 5\text{CH}_3(\text{CH}_2)_4\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_6\text{COOH} + 4\text{H}_2\text{O} + 2\text{H}_2 + \text{CH}_3\text{COOH}$	-141.4
Re.2 $6\text{CH}_3\text{CH}_2\text{OH} + 5\text{CH}_3(\text{CH}_2)_3\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_5\text{COOH} + 4\text{H}_2\text{O} + 2\text{H}_2 + \text{CH}_3\text{COOH}$	-142.4
Re.3 $6\text{CH}_3\text{CH}_2\text{OH} + 5\text{CH}_3(\text{CH}_2)_2\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_4\text{COOH} + 4\text{H}_2\text{O} + 2\text{H}_2 + \text{CH}_3\text{COOH}$	-142.9
Re.4 $6\text{CH}_3\text{CH}_2\text{OH} + 4\text{CH}_3\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_2\text{COOH} + 4\text{H}_2\text{O} + 2\text{H}_2$	-173.9
Re.5 $12\text{CH}_3\text{CH}_2\text{OH} + 3\text{CH}_3\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_4\text{COOH} + 8\text{H}_2\text{O} + 4\text{H}_2$	-316.8
Re.6 $18\text{CH}_3\text{CH}_2\text{OH} + 2\text{CH}_3\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_6\text{COOH} + 12\text{H}_2\text{O} + 6\text{H}_2$	-458.2
Re.7 $12\text{CH}_3\text{CH}_2\text{OH} + 5\text{CH}_3\text{CH}_2\text{COOH} \rightarrow 5\text{CH}_3(\text{CH}_2)_5\text{COOH} + 8\text{H}_2\text{O} + 4\text{H}_2 + 2\text{CH}_3\text{COOH}$	-273.8
Butanol production	
Re.8 $\text{CH}_3(\text{CH}_2)_2\text{COOH} + 2\text{H}_2 \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}_2\text{OH} + \text{H}_2\text{O}$	-50.3
In-situ ethanol production	
Re.9 $\text{C}_6\text{H}_{12}\text{O}_6 \rightarrow 2\text{C}_2\text{H}_5\text{OH} + 2\text{CO}_2$	-241.84

Table S5 Abundance of genes involved in MCFAs, butanol and their key precursors production in different reactors.

KO	Enzyme ID	Control	1Y	4Y	Description
<i>Butanol production via ABE pathway</i>					
K00248	1.3.8.1	0.0117	0.0135	0.0133	butyryl-CoA dehydrogenase
K00100	1.1.1.-	0.0001	0.0005	0.0086	butanol dehydrogenase
<i>Butanol reduction via Butanoate mechanism</i>					
K04073	1.2.1.10	0.0105	0.0069	0.0044	acetaldehyde dehydrogenase
K18366	1.2.1.10	0.0037	0.0033	0.0019	acetaldehyde/propanal dehydrogenase
<i>Chain elongation</i>					
K01961	6.4.1.2	0.0445	0.0572	0.0612	acetyl-CoA carboxylase, biotin carboxylase subunit
K00645	2.3.1.39	0.0377	0.0459	0.0533	[acyl-carrier-protein] S-malonyltransferase
K09458	2.3.1.179	0.0747	0.0808	0.1017	3-oxoacyl-[acyl-carrier-protein] synthase II
K16363	4.2.1.59	0.0042	0.0114	0.0232	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase / 3-hydroxyacyl-[acyl-carrier-protein] dehydratase
K02371	1.3.1.9	0.0096	0.0142	0.0220	enoyl-[acyl-carrier protein] reductase II
K01075	3.1.2.23	0.0073	0.0077	0.0058	4-hydroxybenzoyl-CoA thioesterase
<i>Butyrate production</i>					
K00634	2.3.1.19	0.0037	0.0060	0.0021	phosphate butyryltransferase
K01034	2.8.3.8	0.0019	0.0034	0.0022	acetate CoA/acetoacetate CoA-transferase alpha subunit
K01035	2.8.3.8	0.0017	0.0028	0.0020	acetate CoA/acetoacetate CoA-transferase beta subunit
<i>Ethanol production via yeast</i>					
K00128	1.2.1.3	0.0725	0.0918	0.0931	aldehyde dehydrogenase (NAD+)
<i>Acetyl-CoA production via ethanol reduction</i>					
K19955	1.1.1.-	0.0017	0.0035	0.0065	alcohol dehydrogenase
<i>Acetate production</i>					
K00625	2.3.1.8	0.0190	0.0288	0.0407	phosphate acetyltransferase

Idea conception



Batch tests steps

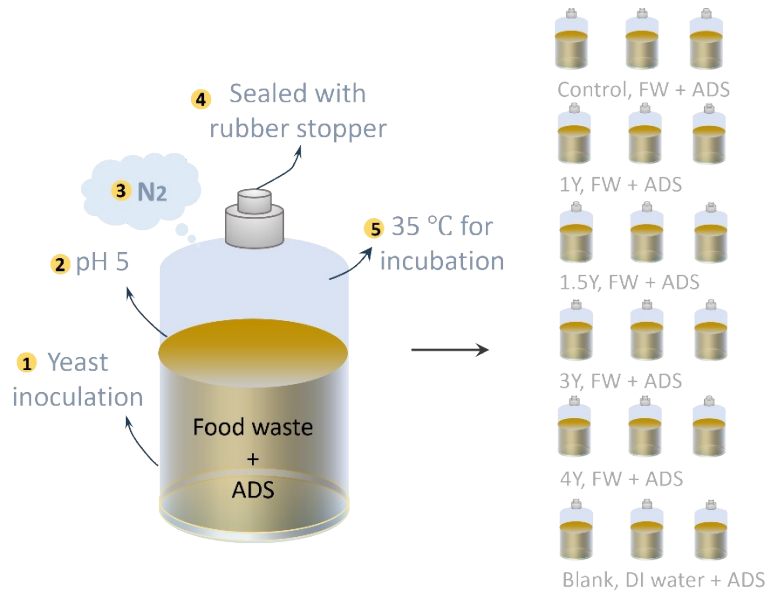


Fig. S1 The flow diagram and experimental design of producing MCFAs and butanol from FW-fed fermentation systems.

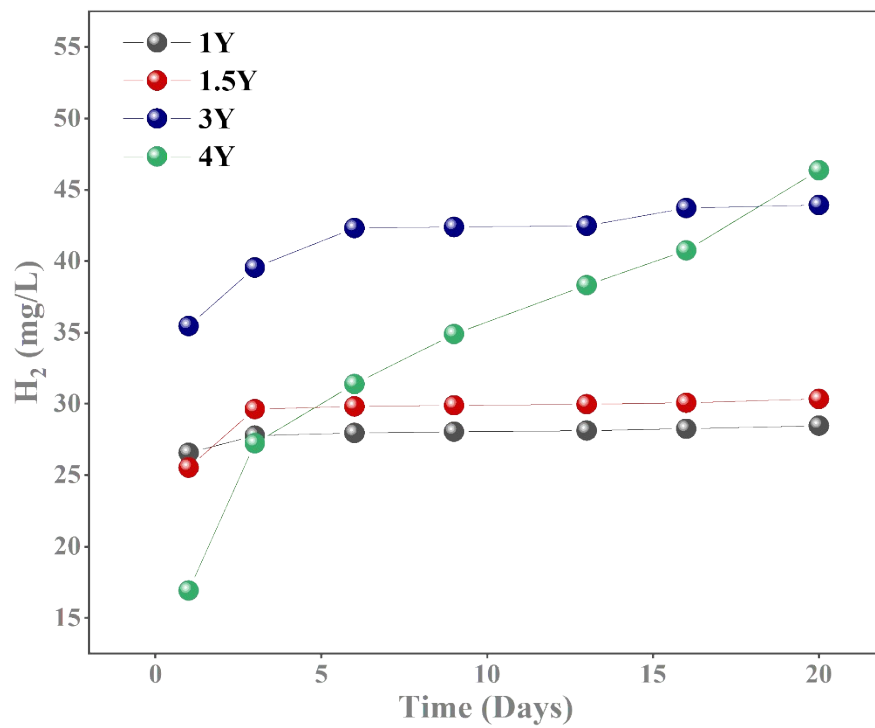


Fig. S2 The accumulated H₂ concentration in the yeast-inoculated systems.

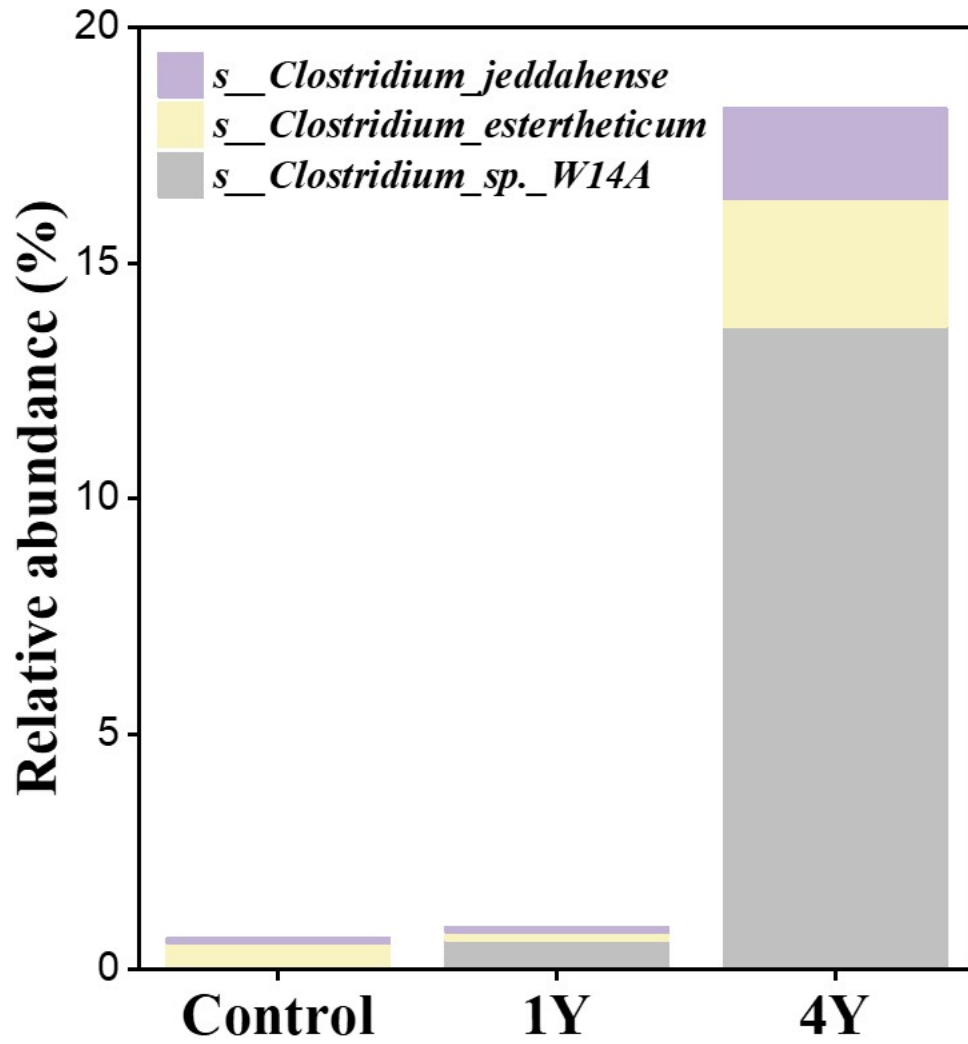


Fig. S3 The relative abundance the *Clostridium* species with the potential to produce butanol. The functions of these microbial species were proposed based on former studies.¹³⁻¹⁵

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