Supplementary Material:

Eco-friendly and sustainable process for converting hydrous bioethanol to butanol

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The view of the mini-pilot unit used for catalysts testing is presented in Figure S1.

Figure S1. Mini-pilot unit used for catalysts testing: a – front view; b- side view

The peripheral equipment of mini-pilot unit used for catalysts testing is consisted of the following parts: high precision liquid pump, for regulating the inlet feed of ethanol and ethanol-water mixtures; mass

flow controllers, necessary for catalyst pre-treatment and during start-up, operation and shut-down procedures; electrical heaters for regulating the reactor inlet temperature as well as the temperature across the reactor; electro-valves ON/OFF placed on the feeding inlets and on the system outlet, as well as manual ball valves; pressure sensors, for measuring the operating pressure of the system; pressure regulator for adjusting the pressure of the system to a desired level; temperature sensors (thermocouple K-type), for measuring the temperature in crucial points of the system; recirculator, for recirculating the cooling liquid; radiator, for cooling down the cooling liquid. The control unit of the system was properly wired with the peripheral equipment based on a Programmable Logic Controller (PLC) permitting conditioning and supervising all process parameters (pressure, temperature, flows etc.) providing reliable and safe operation. In addition, an interface (Supervisory Control and Data Acquisition Software, SCADA) has been developed using INDUSOFT, permitting the operator to observe and regulate the above-mentioned critical parameters of the processes.

The specifications of equipment unit in process simulation have been evaluated using CHEMCAD 7.1.1 simulations software. Distillation columns are simulated using a rigorous multi-stage vapor-liquid equilibrium module. Number of stages and refluxes ratio are adjusted to reach high product purity. Sizing of storage tanks was calculated for allowing 96h of storing. The specifications of each item of equipment is entered into CHEMCAD costing tool or other cost formulas available in the literature for calculating the purchase cost of each item.

Table S1. Summary of purchase cost for main equipment units[a]

Tag No	Equipment unit	Unit size	Heat duty, MW	Remarks	Purchase cost, $K	Ref.
R-01	Adiabatic reactor	V=75m^3	1.8		150	[2]
S-01	Flash drum	D=1.5 m, H=6.5 m			50	
P-01A/B	Pumps	Q=4.5L/sec, Single-stage centrifugal		2 units	9	
P-02A/B		Q=17L/sec, Single-stage centrifugal		2 units	12	
P-03A/B		Q=20L/sec, Single-stage centrifugal		2 units	13	
C-01	Cooling tower&pumps	Q=1,800L/sec	73.8		700	[2]
HE-01	Heat exchangers	A=3,000m^2	31.5		700	
HE-02		A=450m^2	3.8		85	
B-01	Boiler	Q=125 ton/h steam	81.7		1,800	[1]
D-01	Distillation columns	D=3.2m, H=15m	23.9	40 stages, Reflux ratio=0.4	840	
D-02		D=1.5m, H=7.5m	3.0	15 stages, Reflux ratio=0.8	150	
D-03		D=1.7m, H=8m	4.6	20 stages, Reflux ratio=24.7	170	
D-04		D=4.4m, H=12m	41.6	30 stages, Reflux ratio=2.4	1,150	
	Total				**5,829**	

[a] Equipment costs were obtained from CHEMCAD if not stated otherwise.

Table S2. Assumptions for economic model

Parameter	**Valve**
Economic plant life	25 years
Discount rate	10%
Depreciation rate	4%/year
Fixed expenses growth rate	0.5%/year
Plant operation time	8,000h/year
Average income tax rate	35%
Construction time	3 years
1st year	30% of fixed capital
2nd year	40% of fixed capital
3rd year	30% of fixed capital+ 30% of fixed and variable expenses
4th year	85% of design basis production rate

Table S3. Economic parameters for different plant capacities.

Plant scale, Butanol ton/year	**8,000**	**25,000**	**80,000**	**250,000**	**800,000**
Purchase Cost of Equipment (PCE), $K	**1,464**	**2,900**	**9,924**	**11,547**	**23,205**
Total Capital Investment (TCI), $K	**7,823**	**15,495**	**50,650**	**61,699**	**123,990**
Annual expenses	**$K**				
Maintenance	569	1,127	2,265	4,487	9,017
Operating labor	900	900	1,200	1,500	2,100
Laboratory costs	225	225	300	375	525
Supervision	225	225	300	375	525
Plant overheads	450	450	600	750	1,050
Capital charges	284	563	1,133	2,244	4,509
Local taxes	142	282	566	1,122	2,254
Insurance	142	282	566	1,122	2,254
Total fixed expenses	**2,938**	**4,054**	**6,930**	**11,974**	**22,235**
Hydrous Ethanol	7,654	23,919	76,540	239,188	765,400
Catalyst& Operating materials	282	792	2,351	6,992	21,640
Utilities	1,052	3,286	10,516	32,863	105,162
Acetaldehyde credit	-780	-2,438	-7,800	-24,375	-78,000
C5+ alcohol mixture credit	-2,255	-7,048	-22,552	-70,475	225,520
Total variable expenses	**5,953**	**18,513**	59,056	**184,193**	**588,682**
Total direct costs	**8,890**	**22,566**	**65,986**	**196,167**	**610,917**
Indirect costs	**1,778**	**4,513**	**13,197**	**39,233**	**122,183**
Annual production expenses	**10,669**	**27,080**	**79,183**	**235,400**	**733,101**
LCOP, $/kg butanol	**1.54**	**1.22**	**1.09**	**1.02**	**0.98**

References

1. R. Sinnott. Chemical Engineering Design: Chemical Engineering Volume 6. Elsevier, 2005
2. R. Sinnott, G. Towler. Principles, Practice and Economics of Plant and Process Design, Chemical Engineering Design, Elsevier, 2008