Supplementary material captions

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References

Table S1. Stream information of distillation process

	BD-FEED	BD-WATER	BD-1	BD-1BUTENE	BD-2BUTENE	D-BD
Temperature C	37.8	42.1	44.4	42.1	44.1	40.8
Pressure kg/sqcmg	4	3.8	3.958	3.8	3.5	3.5
Vapor Frac	0	0	0	0	0	0
Mass Flow kg/hr	3628.3	3.568	3425.5	199.22	58.234	3367.3
Mass Frac						
1BUTENE	0.01	32 PPM	0.005	0.11	321 PPM	0.005
13BD	0.977	799 PPM	0.983	0.89	0.578	0.99
2BUTENE	0.012	trace	0.012	61 PPB	0.421	0.005
AA	99 PPM	14 PPM	104 PPM	14 PPM	150 PPM	103 PPM
2MPA	trace	trace	trace	trace	3 PPB	trace
MEK	trace	trace	trace	trace	trace	trace
C-HEXANE	trace	trace	trace	trace	trace	trace
H2O	0.001	0.999	trace	456 PPM		
2MPO						
ACETOIN						
23BDO						
HEAVIES (3,5-Xylenol)						
NMP						

Table S2. Stream information of extractive distillation process

	BD-FEED	BD-1	BD-2	BD-3	BD-4	H2O	H2O-NMP1	H2O-NMP2	H2O-NMP3	H2O-NMP4	H2O-NMP5	MK-H2O	MK-NMP	Waste-Water1	Waste-Water2	OFFGAS	ED-BD
Temperature C	37.8	112.1	43.3	41.9	100.3	42.8	120	130.5	130.5	38.7	38.2	38	40	39.7	150.2	57.9	40
Pressure kg/sqcmg	4	5.868	5	0.5	4.5	3.9	4.228	0.528	0.528	6.5	6.5	6.5	6.5	3.7	-0.6	5.5	3.708
Vapor Frac	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	1	0
Mass Flow kg/hr	3628	32774	3555	2019.2	2019.2	222.89	31014	28995	28937	55.243	29215	0.9	2.728	3.41	2.748	73.272	3552.5
Mass Frac																	
1BUTENE	0.01		0.004	0.002	0.002	22 PPM	123 PPM	trace	trace	trace	167 PPB			23 PPM	trace	0.341	0.004
13BD	0.977	0.108	0.992	0.975	0.975	0.009	0.063	3 PPM	3 PPM	4 PPM	73 PPM			0.009	22 PPB	0.242	0.993
2BUTENE	0.012	0	0.003	0.004	0.004	22 PPM	239 PPM	trace	trace	trace	169 PPB			13 PPM	trace	0.406	0.003
AA	99 PPM	48 PPM	100 PPM	182 PPM	182 PPM	99 PPM	50 PPM	41 PPM	41 PPM	43 PPM	42 PPM			78 PPM	509 PPB	17 PPM	100 PPM
2MPA	trace	trace	trace	4 PPB	4 PPB	trace	trace	trace	trace	trace	trace			trace	trace	trace	trace
MEK	trace	6 PPB	trace	26 PPB	26 PPB	trace	8 PPB	7 PPB	7 PPB	8 PPB	7 PPB			trace	trace	trace	trace
C-HEXANE	trace	trace	trace	5 PPB	5 PPB	trace	trace	trace	trace	trace	trace			trace	trace	trace	trace
H2O	0.001	0.134	0.001	0.019	0.019	0.991	0.135	0.143	0.143	0.15	0.15	1		0.991	0.007	0.011	100 PPM
2MPO		71 PPB	trace	30 PPB	30 PPB	trace	77 PPB	80 PPB	80 PPB	81 PPB	80 PPB			trace	78 PPB	trace	trace
ACETOIN		2 PPB	trace	trace	trace	trace	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB				4 PPB	trace	trace
23BDO		trace		trace	trace		trace	trace	trace	trace	trace				trace	trace	
HEAVIES (3,5-Xylenol)		trace		trace	trace		trace	trace	trace	trace	trace				trace	trace	
NMP		0.758		2 PPM	2 PPM	trace	0.801	0.857	0.857	0.85	0.85		1		0.993	4 PPM	

Table S3. Product Specification

Contents	Unit	Minimum	Maximum	Test Method
BD	wt%	99.0		ASTM D 2593
Peroxide	wt ppm		Max. 10	ASTM D 1022
Acetylenes	wt ppm		Max. 400	ASTM D 2593
Carbonyl Compounds as Acetaldehyde	wt ppm		Max. 100	ASTM D 4423
Butadiene Dimer	wt%		Max. 0.2	ASTM D 2426
Non-Volatile Matter	wt%		Max. 0.1	ASTM D 1025
Total Sulfur	wt ppm		Max 10	ASTM D 2784

Table S4. Column Specification of distillation process

Description	Unit	1st Distillation Column	2nd Distillation Column
Number of stages	#	80	56
Pressure	kg/cm^{2}g	3.8	3.5
Feed temperature	℃	37.8	44.4
O/H temperature,	℃	42.1	40.8
BTM temperature	℃	44.4	44.1
Heat Duty	GJ/h	9.05	3.9

Table S5. Column Specification of extractive distillation process

Description	Unit	Extractive distillation column	Stripper	BD Recovery Column	NMP Recovery Column
Number of stages	#	36	15	5	15
Pressure	kg/sqcmg	5.5	4.2	4	0.5
Feed temperature	℃	58.8	112	43.3	120
O/H temperature,	℃	57.9	43.5	41.3	41.9
BTM temperature	℃	112	120	44	130
Heat Duty	GJ/h	5.14	3.78	0.0593	2.43

Table S6. Data Source of Binary Parameters

Data Source	Description
NISTV84	Provided from NIST
APV84	Provided from Aspen plus
R-PCES	Estimated by UNIFAC

Table S7. Binary Parameters (NRTL1) of distillation process

Component i	13BD	13BD	13BD	1BUTENE	1BUTENE	2BUTENE
Component j	H2O	1BUTENE	2BUTENE	2BUTENE	H2O	H2O
Temperature units	C	C	C	C	C	C
Source	NISTV84	APV84	APV84	R-PCES	R-PCES	R-PCES
Property units						
AIJ	7.25398	0	0	0	0	0
AJI	-1.22957	0	0	0	0	0
BIJ	-49.6855	283.4563	12.7828	121.3348	795.8132	900.9591
BJI	2490.16	-223.035	-6.4297	-107.399	1629.561	1599.288
CIJ	0.289695	0.3	0.3	0.3	0.3	0.3
DIJ	0	0	0	0	0	0
EIJ	0	0	0	0	0	0
EJI	0	0	0	0	0	0
FIJ	0	0	0	0	0	0
FJI	0	0	0	0	0	0
TLOWER	6.846	51.67	5	25	25	25
TUPPER	103.825	65.56	65	25	25	25

Table S8. Binary Parameters (NRTL1) of extractive distillation process

Component i	13BD	13BD	13BD	1BUTENE	1BUTENE	2BUTENE	13BD	2BUTENE	H2O
Component j	H2O	1BUTENE	2BUTENE	2BUTENE	H2O	H2O	NMP	NMP	NMP
Temperature units	C	C	C	C	C	C	C	C	C
Source	NISTV84	APV84	APV84	R-PCES	R-PCES	R-PCES	APV86 VLE-RK	APV86 VLE-RK	APV86 VLE-RK
Property units									
AIJ	7.25398	0	0	0	0	0	0	0	7.2111
AJI	-1.22957	0	0	0	0	0	0	0	-2.0976
BIJ	-49.6855	283.4563	12.7828	121.3348	795.8132	900.9591	656.607	635.5333	-2218.79
BJI	2490.16	-223.035	-6.4297	-107.399	1629.561	1599.288	-176.935	66.7867	487.597
CIJ	0.289695	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
DIJ	0	0	0	0	0	0	0	0	0
EIJ	0	0	0	0	0	0	0	0	0
EJI	0	0	0	0	0	0	0	0	0
FIJ	0	0	0	0	0	0	0	0	0
FJI	0	0	0	0	0	0	0	0	0
TLOWER	6.846	51.67	5	25	25	25	15	10	20
TUPPER	103.825	65.56	65	25	25	25	35	30	178.34

Table S9. Binary Parameters (NRTL2) of distillation process

Component i	13BD	13BD	13BD	1BUTENE	1BUTENE	2BUTENE
Component j	H2O	1BUTENE	2BUTENE	2BUTENE	H2O	H2O
Temperature units	C	C	C	C	C	C
Source	APV84	APV84	APV84	R-PCES	R-PCES	R-PCES
Property units						
AIJ	-1.6072	0	0	0	0	0
AJI	-1.6062	0	0	0	0	0
BIJ	2014.5239	283.4563	12.7828	121.3348	795.8132	900.9591
BJI	2014.2203	-223.035	-6.4297	-107.399	1629.561	1599.288
CIJ	0.3	0.3	0.3	0.3	0.3	0.3
DIJ	0	0	0	0	0	0
EIJ	0	0	0	0	0	0
EJI	0	0	0	0	0	0
FIJ	0	0	0	0	0	0
FJI	0	0	0	0	0	0
TLOWER	7	51.67	5	25	25	25
TUPPER	21	65.56	65	25	25	25

Table S10. Binary Parameters (NRTL2) of extractive distillation process

Component i	13BD	13BD	13BD	1BUTENE	1BUTENE	2BUTENE	13BD	2BUTENE	H2O
Component j	H2O	1BUTENE	2BUTENE	2BUTENE	H2O	H2O	NMP	NMP	NMP
Temperature units	C	C	C	C	C	C	C	C	C
Source	APV84	APV84	APV84	R-PCES	R-PCES	R-PCES	APV86 VLE-RK	APV86 VLE-RK	APV86 VLE-RK
Property units									
AIJ	-1.6072	0	0	0	0	0	0	0	7.2111
AJI	-1.6062	0	0	0	0	0	0	0	-2.0976
BIJ	2014.5239	283.4563	12.7828	121.3348	795.8132	900.9591	656.6073	635.5333	-2218.79
BJI	2014.2203	-223.035	-6.4297	-107.399	1629.561	1599.288	-176.9349	66.7867	487.597
CIJ	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
DIJ	0	0	0	0	0	0	0	0	0
EIJ	0	0	0	0	0	0	0	0	0
EJI	0	0	0	0	0	0	0	0	0
FIJ	0	0	0	0	0	0	0	0	0
FJI	0	0	0	0	0	0	0	0	0
TLOWER	7	51.67	5	25	25	25	15	10	20
TUPPER	21	65.56	65	25	25	25	35	30	178.34

The total capital investment including the inside battery limits investment (ISBL) and the outside battery limits investment (OSBL) is used to analyze the economic feasibility of the process, as shown in Table S11. The total capital investment is calculated by the factorial method. ISBL means the instantaneous investment for the main process to manufacture the products. The items of the ISBL consist of the process equipment, building, piping, instrument and control, electrical system, lagging and painting, and civil. The purchased cost (C_P^0) is estimated by Turton's method (Eq.S1), and the other costs are calculated by Towler's method (Eq.S2), as shown in Table S11, respectively.[1,2]

$$log_{10}C_P^0 = K_1 + K_2 log_{10}(A) + K_3(log_{10}(A))^2 \quad \text{(S1)}$$

where A is the capacity or size parameter for the equipment. C_P^0 is the purchased cost and the value for K_1, K_2 and K_3 are given in Turton's method.

$$\mathrm{C} = \sum_{i=1}^{i=M} C_{e,i,CS}((1+f_p)f_m + (f_{er} + f_{el} + f_i + f_c + f_s + f_l)) \quad \text{(S2)}$$

where $C_{e,i,CS}$ is the purchased cost of the equipment i in carbon steel and is equal to C_P^0. The information for each factor is specified in Table S11. f_m is (purchased cost in exotic material) / (purchased cost in carbon steel) and the value is 1.3 in this analysis, reflecting the cost of using stainless steel.

OSBL represents the necessary and auxiliary costs to operate the main process. The items of OSBL typically consist of a storage system, a steam generation unit, a cooling water system and a water treatment system. In this analysis, OSBL is calculated to be 40% of ISBL by factorial method. In addition, an offsite cost, a contingency, a working capital, a design and engineering are estimated in Table S11. Then, Table S12 shows the revenue and utility summary of the conventional and the alternative processes with no consideration of the cost of several raw materials such as 2,3-BDO, catalyst, and cyclohexane, introducing to preceding units. In the case of the alternative process, the cost of NMP is \$ 3.33/kg and water are considered as raw material.[3] When the annual cost of 1,3-BD is calculated, \$ 2.5/kg applied for its price per weight as the average value of it for 3 years (2013 – 2015).

Table S11. ISBL, OSBL, Total Capital Cost and Total fixed capital investment of 1,3-BD purification part of the distillation process and extractive distillation processes [1,2].

Contents		**Factor**	**Conventional process [M$]**	**Alternative process [M$]**
ISBL	Purchased equipment, $C_{e,i,CS}(C_P^0)$	1	0.526	1.07
	Equipment erection, f_{er}	0.3	0.158	0.321
	Instrumentation and controls, f_i	0.3	0.158	0.321

	Piping, f_p	0.8	0.421	0.856
	Electrical, f_{el}	0.2	0.105	0.214
	Structures and Buildings, f_s	0.2	0.105	0.214
	Civil, f_c	0.3	0.158	0.321
	Lagging and Paint, f_l	0.1	0.053	0.101
	Total		1.97	4.01
OSBL		40% of ISBL	0.842	1.72
Design and Engineering		30% of ISBL	0.590	1.20
Contingency		10% of ISBL	0.197	0.401

Total capital cost (TCC)		3.60	7.34
Working capital	20% of TCC	0.719	1.47
Total fixed capital investment		4.32	8.81

Table S12. Revenue and Utility Summary of the distillation process and extractive distillation processes [2].

		Conventional process		Alternative process	
Raw materials		**Mass flow rate [kg/h]**	**Annual cost [M$]**	**Mass flow rate [kg/h]**	**Annual cost [M$]**
	NMP	-	-	2.728	0.727
	Water	-	-	0.9	0.00482
	Total	-	-		0.731
Utility		**Flow rate [GJ/h]**	**Annual cost, [M$]**	**Flow rate [GJ/h]**	**Annual cost, [M$]**
	Cooling water (0.354 $/GJ)	12.93	0.037	12.07	0.034
	LP steam (13.28 $/GJ)	12.93	1.37	12.83	1.36

	Electricity (16.8 $/GJ)	0	0	0.22	0.0296
	Total		1.41		1.42
Revenue		**Mass flow rate [kg/h]**	**Annual cost, [M$]**	**Mass flow rate [kg/h]**	**Annual cost, [M$]**
	1,3-BD	3,367	80.8	3,553	85.3
		Volumetric flow rate [m^3/h]	**Annual cost, [M$]**	**Volumetric flow rate [m^3/h]**	**Annual cost, [M$]**
	Fuel	0.436	1.92	-	-
	Total		82.7		85.3

Reference

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