Supporting information

What is the best green propylene production pathway? : Technical, economic, and environmental assessment

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1. Process modeling

This work conducts a comprehensive analysis, including technical, economic, and environmental aspects, simultaneously, of the green propylene production via indirect and direct methanol (MeOH) synthesis based on the process modeling using Aspen Plus®. For process modeling of the MeOH production and MeOH to propylene (MTP) was simulated based on the process developed in the literature [1,2]. Table S1 shows the main flow results for green propylene production process modeling, including MeOH synthesis and MTP sections. In addition, environmental impact assessment was performed using GREET® database based on process simulation results. Fig. S1 and Fig. S2 represent the detailed system boundary of environmental impact assessment for both MTP pathways.

Table S1. Main flow results for green propylene production process modeling

	H_2	CO_2	1	2	3	4
Temperature/ C	179.83	159.85	63.12	210	284.51	284.51
Pressure/ bar	75	75	75	75	75	75
Molar Vapor Fraction	1	1	1	1	1	1
Molar Liquid Fraction	0	0	0	0	0	0
Mole Flows/ kmol hr^{-1}	992.12	332	7880.89	7880.89	7268.32	4360.8
Mole Fractions						
CH_3OH (MeOH)	0.000	0.000	0.00321	0.00321	0.0456	0.0456
CO	0.000	0.000	0.0311	0.0311	0.0342	0.0342
CO_2	0.000	1.000	0.124	0.124	0.0920	0.0920
H_2	1.000	0.000	0.841	0.841	0.785	0.785

H_2O	0.000	0.000	0.000674	0.000674	0.0433	0.0433
C_2H_6O (DME)	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_4	0.000	0.000	0.000	0.000	0.000	0.000
C_3H_6 (Propylene)	0.000	0.000	0.000	0.000	0.000	0.000
C_4H_8	0.000	0.000	0.000	0.000	0.000	0.000
C_5H_{10}	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_6	0.000	0.000	0.000	0.000	0.000	0.000

(Continuous)

	5	6	7	8	MeOH	9
Temperature/ C	93.10	92.87	70	84.34	64.05	82.23
Pressure/ bar	75	75	1.2	1.1	1	75

Molar Vapor Fraction	0.943	0.943	0.00861	0	1	0.932
Molar Liquid Fraction	0.0569	0.0572	0.991	1	0	0.0676
Mole Flows/ kmol hr^{-1}	4360.8	2907.33	612.521	375.682	236.839	2907.33
Mole Fractions						
CH_3OH (MeOH)	0.0456	0.0456	0.493	0.179	0.992	0.0456
CO	0.0342	0.0342	0.000	0.000	0.000	0.0342
CO_2	0.0920	0.0920	0.003	0.000	0.00699	0.0342
H_2	0.785	0.785	0.000	0.000	0.000373	0.785
H_2O	0.0433	0.04333	0.504	0.821	0.001	0.0433
C_2H_6O (DME)	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_4	0.000	0.000	0.000	0.000	0.000	0.000
C_3H_6 (Propylene)	0.000	0.000	0.000	0.000	0.000	0.000

C_4H_8	0.000	0.000	0.000	0.000	0.000	0.000
C_5H_{10}	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_6	0.000	0.000	0.000	0.000	0.000	0.000

(Continuous)

	10	11	12	13	Recycle	14
Temperature/ C	40	33	40	40	40	79.43
Pressure/ bar	75	1.2	75	75	75	1.2
Molar Vapor Fraction	0	1	1	1	1	1
Molar Liquid Fraction	1	0	0	0	0	0
Mole Flows/ kmol hr^{-1}	645.026	32.505	6623	66.23	6556.77	236.839
Mole Fractions						

CH_3OH (MeOH)	0.474	0.118	0.00386	0.00386	0.00386	0.992
CO	0.001	0.0215	0.0374	0.0374	0.0374	0.000
CO_2	0.001	0.0215	0.0986	0.0986	0.0986	0.00699
H_2	0.0198	0.390	0.859	0.859	0.859	0.000373
H_2O	0.480	0.0249	0.000811	0.000811	0.000811	0.001
C_2H_6O (DME)	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_4	0.000	0.000	0.000	0.000	0.000	0.000
C_3H_6 (Propylene)	0.000	0.000	0.000	0.000	0.000	0.000
C_4H_8	0.000	0.000	0.000	0.000	0.000	0.000
C_5H_{10}	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000
C_2H_6	0.000	0.000	0.000	0.000	0.000	0.000

(Continuous)

	15	16	17	Water	18
Temperature/ C	40	420	90	90	90
Pressure/ bar	1	7	7	7	7
Molar Vapor Fraction	1	1	0.205	1	0
Molar Liquid Fraction	0	0	0.795	0	1
Mole Flows/ kmol hr^{-1}	1.033	235.806	314.227	101.588	212.639
Mole Fractions					
CH_3OH (MeOH)	0.355	0.995	0.0600	0.185	0.000
CO	0.00557	0.000	0.00853	0.0264	0.000
CO_2	0.562	0.00456	0.00412	0.0127	0.000
H_2	0.0777	0.000	0.013	0.0417	0.000

H_2O	0.000	0.001	0.677	0.000	1.000
C_2H_6O (DME)	0.000	0.000	0.000425	0.00131	0.000
C_2H_4	0.000	0.000	0.074	0.230	0.000
C_3H_6 (Propylene)	0.000	0.000	0.106	0.327	0.000
C_4H_8	0.000	0.000	0.051	0.159	0.000
C_5H_{10}	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.00528	0.0163	0.000
C_2H_6	0.000	0.000	0.000425	0.00116	0.000

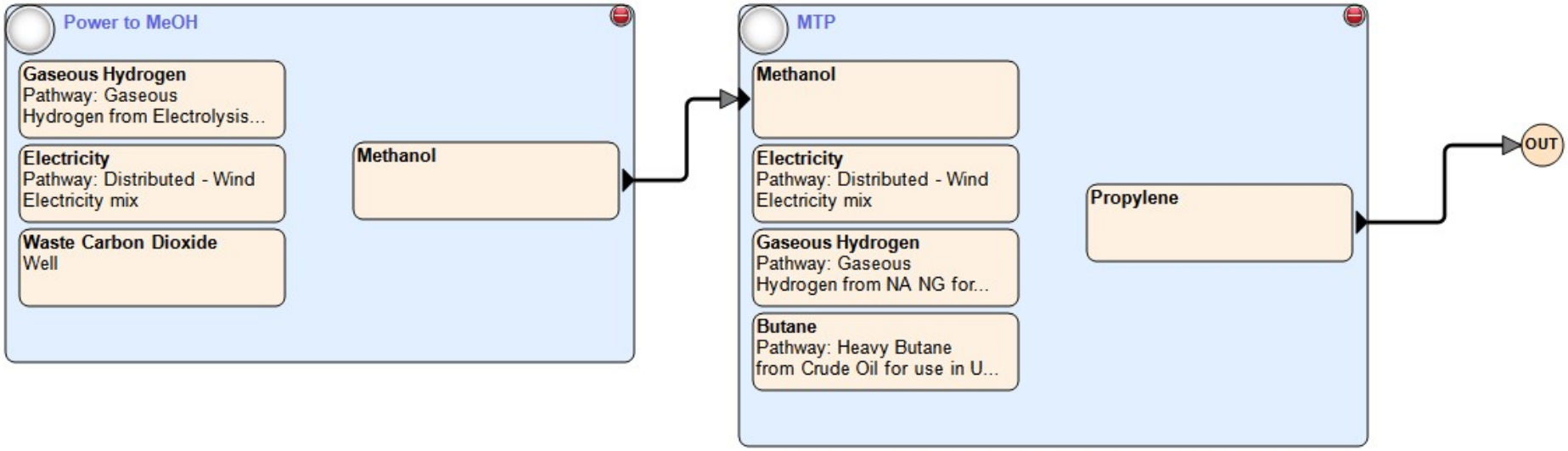

Fig. S1. Detailed system boundary of environmental impact assessment for green propylene production via indirect MeOH synthesis.

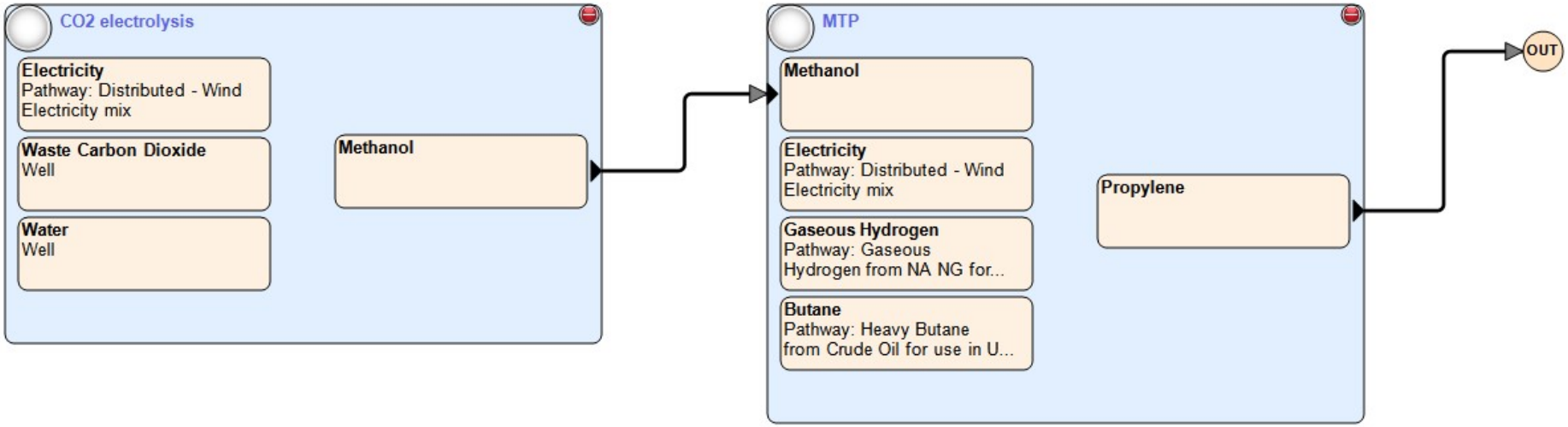

Fig. S2. Detailed system boundary of environmental impact assessment for green propylene production via direct MeOH synthesis.

Reference

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[2] A. T. Najafabadi, S. Fatemi, M. Sohrabi and M. Salmasi, *J. Ind. Eng. Chem.*, 2012, **18**, 29–37.