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APPENDIX

A1 DWSIM을 이용한 가상 공정 설계

A1.1 DWSIM Flow Table

Table A1 Flow table for DRM+FT process

Stream	Type	T [ºC]	P [bar]	Mass flow [ton/h]
ch_4 feedstock	In	50	0.86	16.04
CO_2 feedstock	In	50	0.86	44.01
DRM reactor	Inlet	800	0.86	66.72
	Outlet	800	0.76	66.72
FT reactor	Inlet	220	26.7	109.4
	Outlet	220	26.6	109.4
HC reactor	Inlet	360	20	6.58
	Outlet	362	19.9	6.58
Liquid product	Light naphtha	90	1.01	2.36
	e-Kerosene	90	1.01	7.1
	FT wax	326	1.01	4.17
Gas product	CO	191	30	28.01
	Light gas	220	26.7	1.87

Table A2 Flow table for WE&RWGS+FT process

Stream	Type	T [ºC]	P [bar]	Mass flow [ton/h]
Water feedstock	In	25	1.01	90.08
CO_2 feedstock	In	-20	26.7	44.01
PEM unit	Inlet	80.1	26.7	90.08
	Outlet	80.1	26.6	75.95
	Outlet (H_2O)	80.1	26.6	14.12
RWGS reactor	Inlet	800	26.4	76.18
	Outlet	800	26.3	76.18
FT reactor	Inlet	220	26.7	101.69
	Outlet	220	26.6	101.69
HC reactor	Inlet	360	20	3.07
	Outlet	362	19.9	3.07
Liquid product	Light Naphtha	90	1.01	1.76
	e-Kerosene	90	1.01	5.19
	FT wax	326	1.01	2.77
Gas product	H_2	80	26.3	2.22
	O_2	73.9	16.7	66.45
	CO	220	26.6	2.94
	Light gas	220	26.6	1.5

Table A1, A2는 각 공정에 적용된 상세 온도, 압력, 유량 조건을 정리하였다. Heat Exchanger, Heater, Cooler, Compressor, Pump의 입구 및 출구 정보는 생략하였다.

A1.2 DWSIM Reactor별 세부 반응식

A1.2.1 FT Reactor 반응식

$$CO + n^{H_2}H_2 \rightarrow \Sigma_i n_i C_i H_{2i+2} + H_2O,\ \ \forall i \in [1, 22] \quad (12)$$

where $n_1 = (1-\alpha)^2\alpha^{i-1}\ \forall i \in [1, 111]$

$$n^{H_2} = \Sigma_i (i+1)n_i + 1 = 3 - \alpha\ \forall i \in [1, 111] \quad (13)$$

식(12) 및 식(13)는 단일 사슬 성장 확률(α) 값을 갖는 Anderson-Shulz-Flory (ASF) 분포를 따른다고 가정하였을 때의 반응식이다. 통계적으로 존재 가능한 모든 파라핀의 분포를 계산하였으며, C23 이상의 모든 무거운 파라핀을 하나의 대표 물질인 Docosane (C22)으로 일괄 처리하여 모델링하였다[10].

A1.2.2 HC Reactor 반응식

$$C_{22}H_{46} + n^{H_2}H_2 \rightarrow \Sigma_i n_i C_i H_{2i+2},\ \ \forall i \in [1, 21] \quad (14)$$

식(14)은 FT 공정에서 생성된 무거운 왁스(Wax)를 수소와 반응시켜 더 가벼운 생성물로 전환하는 HC 공정의 반응식이다. 앞서 대표 물질인 Docosane을 반응물로 가정하여 설계하였다.

A2. LCI

Tables A3 및 A4는 각 공정의 LCI를 보여주고 있다. 1 kg의 e-kerosene 생산에 필요한 자원의 양과 배출되는 물질의 양이 정리되어 있다.

Table A3 Life cycle inventory for DRM+FT process

Functional unit: [1 kg of e-kerosene]	1 kg
Avoided products [kg]	
Light Naphtha (C5-C7)	0.3384
FT Wax (C17-C21)	0.5393
Methane	0.0385
Ethane	0.0636
Propane	0.0816
Butane	0.0950
Carbon monoxide	5.3700
Inputs from nature [kg]	
Cobalt	1.27.E-08
Nickel	1.00.E-05
Platinum	4.08.E-08
Cooling water	2040.0299
Inputs from Technosphere: Materials/fuels [kg]	
Methane	3.0756
Carbon dioxide, liquified	8.4374
Alumina, at plant	1.41.E-04
Zeolite, powder	4.04.E-06
Inputs from Technosphere: electricity/heat [kWh]	
Electricity	3.3651
Heat	15.8253
Emissions to air [kg]	
Hydrogen	1.1838
Emissions to water [kg]	
Waste water	3.0017

Table A4 Life cycle inventory for WE&RWGS+FT process

Functional unit: [1kg of e-kerosene]	1 kg
Avoided products [kg]	
Light Naphtha (C5-C7)	0.3394
FT wax (C17-C21)	0.5323
Methane	0.0400
Ethane	0.0661
Propane	0.0847
Butane	0.0986
Carbon monoxide	0.5677
Inputs from nature [kg]	
Cobalt	1.27E-08
Nickel	4.87E-07
Platinum	4.08E-08
Cooling water	3616.8125
Inputs from Technosphere: Materials/fuels [kg]	
Carbon dioxide, liquified	8.4720
Alumina, at plant	5.51.E-05
Zeolite, powder	4.04.E-06
Ultra-pure water (UPW)	17.3402
Inputs from TECHNOSPHERE: electricity/heat [kWh]	
Electricity	81.2329
Heat	16.0978
Emissions to air [kg]	
Hydrogen	0.5528
Oxygen	12.7910
Emissions to water [kg]	
Waste water	9.5560