

Advancement of Methanol Purity in CO₂ Hydrogenation Process Through Design Optimization, Multistage Compression Simulation, and Purification Model Refinement

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Table S1. Mass balance and energy balance of the basic (unmodified) methanol production process through the hydrogenation CO₂ process calculated using ASPEN HYSYS

Name	Feed CO2	Feed H2	Mix 101	Rec	Prefeed	MIX2
Vapour Fraction	1	1	1	1	0,99932247	1
Temperature [F]	105,8	105,8	84,51496761	139,0611334	132,0444887	143,5994778
Pressure [psia]	616,410225	616,410225	616,410225	607,707963	607,707963	652,66965
Molar Flow [lbmole/hr]	3000	6014,1488	9014,1488	76236,0399	85250,1887	85250,1887
Mass Flow [kg/h]	59888,00795	5499,648088	65387,65604	1513152,907	1578540,563	1578540,563
Liquid Volume Flow [m3/h]	72,56205826	78,72486278	151,286921	1833,740675	1985,027596	1985,027596
Heat Flow [kJ/h]	-537569217,7	1339760,902	-536229456,8	-13514916205	-14051145662	-14042629418
Name	Feed Reactor	Steam(in)	Vapor P	Outlet reactor	Product	B1
Vapour Fraction	1	1	1	0	0,927593059	1
Temperature [F]	212	662	514,76	514,76	69,8	139,0386079
Pressure [psia]	616,410225	14,69231901	609,15834	609,15834	607,707963	607,707963
Molar Flow [lbmole/hr]	85250,1887	22046	81240,75616	0	81240,75616	76939,91005
Mass Flow [kg/h]	1578540,563	180151,0048	1578539,927	0	1578539,927	1527229,378
Liquid Volume Flow [m3/h]	1985,027596	180,514557	1910,845606	0	1910,845606	1850,765208
Heat Flow [kJ/h]	-13970061279	-2304741266	-13730792083	0	-14267739982	-13642196315
Name	B2	Steam(out)	MEOH	WATER		
Vapour Fraction	0	1	1	0		
Temperature [F]	139,0386079	295,5482239	329,1749304	357,0823259		
Pressure [psia]	607,707963	11,06637651	146,488077	147,0682278		
Molar Flow [lbmole/hr]	4300,846111	22046	4240,853196	59,99291529		
Mass Flow [kg/h]	51310,54883	180151,0048	50819,54761	491,0012146		
Liquid Volume Flow [m3/h]	60,08039865	180,514557	59,58796243	0,492436217		
Heat Flow [kJ/h]	-526841171,4	-2377309405	-437233703,3	-7453240,273		
Name	Out 1	Out 2	OK 2	Out 3	OK3	Out 4
Vapour Fraction	1	1	1	1	1	1
Temperature [F]	109,4099104	105,8	127,4183537	105,8	117,7372075	105,8
Pressure [psia]	630	615	700	697,8244345	750	735
Molar Flow [lbmole/hr]	2050	2050	2050	2050	2050	2050
Mass Flow [kg/h]	40923,4721	40923,4721	40923,4721	40923,4721	40923,4721	40923,4721
Liquid Volume Flow [m3/h]	49,58407315	49,58407315	49,58407315	49,58407315	49,58407315	49,58407315
Heat Flow [kJ/h]	-367283806	-367334106	-367002602,8	-367630429,4	-367455061,1	-367771486,4
Name	input CO2	input H2	steam in	out vap abs	out liq abs	out H3
Vapour Fraction	1	1	0	1	0	8,05E-04
Temperature [F]	109,1215052	109,13	186,8	186,7236568	176,3193225	176
Pressure [psia]	750	750	200	200	200	185
Molar Flow [lbmole/hr]	2050	6014,1488	2204,6	184,0900965	6262,593434	6262,593434
Mass Flow [kg/h]	40923,4721	5499,648088	18015,10048	3567,922136	64622,70771	64622,70771
Liquid Volume Flow [m3/h]	49,58407315	78,72486278	18,0514557	4,307453885	72,41433372	72,41433372
Heat Flow [kJ/h]	-367723696,5	1507553,781	-281252208,5	-32095967,55	-765141897,5	-765183491,9
Name	VLV	top	bottom	out H2		
Vapour Fraction	5,38E-03	1	0	4,74E-03		
Temperature [F]	147,1215964	147,1215964	147,1215964	158		
Pressure [psia]	557,707963	557,707963	557,707963	542,707963		
Molar Flow [lbmole/hr]	4265,029865	22,94633473	4242,083531	4242,083531		
Mass Flow [kg/h]	50630,4159	454,8865316	50175,52937	50175,52937		
Liquid Volume Flow [m3/h]	59,22159766	0,55126575	58,67033191	58,67033191		
Heat Flow [kJ/h]	-521098011,9	-4057515,254	-517040496,7	-515987268,1		

Table S1. Continued

Komposisi						
Name	Feed CO2	Feed H2	Mix 101	Rec	Prefeed	MIX2
Comp Mole Frac (Hydrogen)	0	1	0,667189874	0	7,05E-02	7,05E-02
Comp Mole Frac (CO2)	1	0	0,332810126	0,982319761	0,913642183	0,913642183
Comp Mole Frac (Methanol)	0	0	0	1,48E-02	1,32E-02	1,32E-02
Comp Mole Frac (H2O)	0	0	0	2,90E-03	2,59E-03	2,59E-03
Name	Feed Reactor	Steam(in)	Vapor P	Outlet reactor	Product	B1
Comp Mole Frac (Hydrogen)	7,05E-02	0,00E+00	3,69E-102	0,00E+00	3,69E-102	0
Comp Mole Frac (CO2)	0,913642183	0	0,934056449	0,934056505	0,934056449	9,83E-01
Comp Mole Frac (Methanol)	1,32E-02	0,00E+00	3,85E-02	3,85E-02	3,85E-02	1,43E-02
Comp Mole Frac (H2O)	2,59E-03	1,00E+00	2,74E-02	2,74E-02	2,74E-02	2,99E-03
Name	B2	Steam(out)	MEOH	WATER		
Comp Mole Frac (Hydrogen)	0	0	0	0		
Comp Mole Frac (CO2)	6,43E-02	0	6,52E-02	1,00E-30		
Comp Mole Frac (Methanol)	4,72E-01	0,00E+00	4,78E-01	2,00E-03		
Comp Mole Frac (H2O)	4,64E-01	1,00E+00	4,57E-01	9,98E-01		
Name	Out 1	Out 2	OK 2	Out 3	OK3	Out 4
Comp Mole Frac (Hydrogen)	0	0	0	0	0	0
Comp Mole Frac (CO2)	1	1	1	1	1	1
Comp Mole Frac (Methanol)	0	0	0	0	0	0
Comp Mole Frac (H2O)	0	0	0	0	0	0
Name	input CO2	input H2	steam in	out vap abs	out liq abs	out H3
Comp Mole Frac (Hydrogen)	0	1	0	0	0	0
Comp Mole Frac (CO2)	1	0	0	0,95070183	9,72E-03	9,72E-03
Comp Mole Frac (Methanol)	0	0	0	9,69E-28	0,319472916	0,319472916
Comp Mole Frac (H2O)	0	0	1	4,93E-02	0,670808363	0,670808363
Name	VLV	top	bottom	out H2		
Comp Mole Frac (Hydrogen)	0	0	0	0		
Comp Mole Frac (CO2)	6,06E-02	0,978878938	5,56E-02	5,56E-02		
Comp Mole Frac (Methanol)	0,469194084	1,73E-02	0,471638281	0,471638281		
Comp Mole Frac (H2O)	0,470234036	3,79E-03	0,472757158	0,472757158		
Energy Stream						
Name	Q1	E1	E2	E3	Qc	Qr
Heat Flow [kJ/h]	8516243,334	239269196,1	536947899	98702496,04	2264748926	2346907279

Table S2. Mass balance and energy balance of the basic (modified) methanol production process through the hydrogenation CO₂ process calculated using ASPEN HYSYS

Name	Feed CO2	Feed H2	Mix 101	Rec	Prefeed	MIX2
Vapour Fraction	1	1	1	1	0,99905103	1
Temperature [F]	105,8	105,8	85,57120415	147,2297036	139,4126954	165,5
Pressure [psia]	616,410225	616,4	750	607,707963	607,707963	610
Molar Flow [lbmole/hr]	2050	6014,1488	8064,1488	67495,6448	75559,7936	75559,7936
Mass Flow [kg/h]	40923,4721	5499,648088	46423,12019	1338368,751	1384791,871	1384791,871
Liquid Volume Flow [m3/h]	49,58407315	78,72486278	128,3089359	1621,917728	1750,226663	1750,226663
Heat Flow [kJ/h]	-367338965,4	1339759,18	-366216142,8	-11944026889	-12310243032	-12285765863
Name	Feed Reactor	Vapor P	Outlet reactor	Product	B1	B2
Vapour Fraction	1	1	0	0,916843774	1	0
Temperature [F]	212	514,76	514,76	69,8	147,3689492	147,3689492
Pressure [psia]	616,410225	609,15834	609,15834	607,707963	607,707963	607,707963
Molar Flow [lbmole/hr]	75559,7936	71550,36107	0	71550,36107	67285,3312	4265,029865
Mass Flow [kg/h]	1384791,871	1384791,235	0	1384791,235	1334160,819	50630,4159
Liquid Volume Flow [m3/h]	1750,226663	1676,044673	0	1676,044673	1616,823076	59,22159766
Heat Flow [kJ/h]	-12245155857	-12040634311	0	-12525887876	-11906087368	-521098011,9
Name	B2A	Pure feed	compressed	MEOH	WATER	Input MIX
Vapour Fraction	1	1	1	1	0	1
Temperature [F]	147,3689492	147,3689492	147,3671245	279,0325935	356,6259448	155,0677668
Pressure [psia]	607,707963	607,707963	607,707963	146,488077	147,0682278	765
Molar Flow [lbmole/hr]	67285,3312	0	67285,3312	2021,791027	4240,802407	6014,1488
Mass Flow [kg/h]	1334160,819	0	1334160,819	29586,71234	35035,99537	5499,648088
Liquid Volume Flow [m3/h]	1616,823076	0	1616,823076	37,08544903	35,32888469	78,72486278
Heat Flow [kJ/h]	-11906087368	0	-11906088947	-186405730,8	-525918280,5	-3511751,164
Name	Out 1	Out 2	OK 2	Out 3	OK3	Out 4
Vapour Fraction	1	1	1	1	1	1
Temperature [F]	109,4099104	105,8	127,4183537	105,8	117,7372075	105,8
Pressure [psia]	630	615	700	697,8244345	750	735
Molar Flow [lbmole/hr]	2050	2050	2050	2050	2050	2050
Mass Flow [kg/h]	40923,4721	40923,4721	40923,4721	40923,4721	40923,4721	40923,4721
Liquid Volume Flow [m3/h]	49,58407315	49,58407315	49,58407315	49,58407315	49,58407315	49,58407315
Heat Flow [kJ/h]	-367283806	-367334106	-367002602,8	-367630429,4	-367455061,1	-367771486,4
Name	input CO2	input H2	steam in	out vap abs	out liq abs	out H3
Vapour Fraction	1	1	0	1	0	8,05E-04
Temperature [F]	109,1215052	109,13	186,8	186,7236568	176,3193225	176
Pressure [psia]	750	750	200	200	200	185
Molar Flow [lbmole/hr]	2050	6014,1488	2204,6	184,0900965	6262,593434	6262,593434
Mass Flow [kg/h]	40923,4721	5499,648088	18015,10048	3567,922136	64622,70771	64622,70771
Liquid Volume Flow [m3/h]	49,58407315	78,72486278	18,0514557	4,307453885	72,41433372	72,41433372
Heat Flow [kJ/h]	-367723696,5	1507553,781	-281252208,5	-32095967,55	-765141897,5	-765183491,9
Name	VLV	top	bottom	out H2		
Vapour Fraction	5,38E-03	1	0	4,74E-03		
Temperature [F]	147,1215964	147,1215964	147,1215964	158		
Pressure [psia]	557,707963	557,707963	557,707963	542,707963		
Molar Flow [lbmole/hr]	4265,029865	22,94633473	4242,083531	4242,083531		
Mass Flow [kg/h]	50630,4159	454,8865316	50175,52937	50175,52937		
Liquid Volume Flow [m3/h]	59,22159766	0,55126575	58,67033191	58,67033191		
Heat Flow [kJ/h]	-521098011,9	-4057515,254	-517040496,7	-515987268,1		

Table S2. Continued

Komposisi						
Name	Feed CO2	Feed H2	Mix 101	Rec	Prefeed	MIX2
Comp Mole Frac (Hydrogen)	0	1	0,745788421	0	7,96E-02	7,96E-02
Comp Mole Frac (CO2)	1	0	0,254211579	0,97968007	0,902254159	0,902254159
Comp Mole Frac (Methanol)	0	0	0	1,66E-02	1,49E-02	1,49E-02
Comp Mole Frac (H2O)	0	0	0	3,68E-03	3,28E-03	3,28E-03
Name	Feed Reactor	Vapor P	Outlet reactor	Product	B1	B2
Comp Mole Frac (Hydrogen)	7,96E-02	3,72E-102	0	3,72E-102	0	0
Comp Mole Frac (CO2)	0,902254159	0,924795078	0,924795173	0,924795078	0,979575781	6,06E-02
Comp Mole Frac (Methanol)	1,49E-02	4,37E-02	4,37E-02	4,37E-02	1,67E-02	0,469194084
Comp Mole Frac (H2O)	3,28E-03	3,15E-02	3,15E-02	3,15E-02	3,68E-03	0,470234036
Name	B2A	Pure feed	compressed	MEOH	WATER	Input MIX
Comp Mole Frac (Hydrogen)	0	0	0	0	0	1
Comp Mole Frac (CO2)	0,979575781	0,979575781	0,979575781	3,01E-02	4,36E-24	0
Comp Mole Frac (Methanol)	1,67E-02	1,67E-02	1,67E-02	0,959896449	1,42E-02	0
Comp Mole Frac (H2O)	3,68E-03	3,68E-03	3,68E-03	1,00E-02	0,985847264	0
Name	Out 1	Out 2	OK 2	Out 3	OK3	Out 4
Comp Mole Frac (Hydrogen)	0	0	0	0	0	0
Comp Mole Frac (CO2)	1	1	1	1	1	1
Comp Mole Frac (Methanol)	0	0	0	0	0	0
Comp Mole Frac (H2O)	0	0	0	0	0	0
Name	input CO2	input H2	steam in	out vap abs	out liq abs	out H3
Comp Mole Frac (Hydrogen)	0	1	0	0	0	0
Comp Mole Frac (CO2)	1	0	0	0,95070183	9,72E-03	9,72E-03
Comp Mole Frac (Methanol)	0	0	0	9,69E-28	0,319472916	0,319472916
Comp Mole Frac (H2O)	0	0	1	4,93E-02	0,670808363	0,670808363
Name	VLV	top	bottom	out H2		
Comp Mole Frac (Hydrogen)	0	0	0	0		
Comp Mole Frac (CO2)	6,06E-02	0,978878938	5,56E-02	5,56E-02		
Comp Mole Frac (Methanol)	0,469194084	1,73E-02	0,471638281	0,471638281		
Comp Mole Frac (H2O)	0,470234036	3,79E-03	0,472757158	0,472757158		

Energy Stream						
Name	E1	E2	E3	E4	Qc	Qr
Heat Flow [kJ/h]	204521546,4	485253565,6	98702496,04	1578,115066	574314821,4	627185813,9
Name	EK1	EK2	Ec1	EK3	Ec2	EK4
Heat Flow [kJ/h]	2171991,984	55159,4023	50300,01874	331503,1675	627826,5688	175368,317
Name	Ec3	EK5	Ec4	eK6	eH1	eH3
Heat Flow [kJ/h]	316425,2986	47789,86115	2004197,384	24477168,9	40610005,48	-41594,39686
Name	eH2					
Heat Flow [kJ/h]	1053228,512					