Ex-ante Assessment of Life cycle Inherent Safety (ExALIS) of Industrial Value Chains

SUPPLEMENTARY MATERIAL

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Process Flow Diagram (PFD) information

Table S1.Details of the nodes of the biomethane-based value chain.

NODE	DESCRIPTION	T	P	CH_4	CO_2	H_2S	H_2O	O_2	N_2	FLOW RATE	INVENTORY
		°C	bar	wt%	wt%	wt%	wt%	wt%	wt%	kg/s	kg
D01, D02	Tubular Reactor	55.00	1.10	56.00	42.00	2.00	0.00	0.00	0.00	0.00	31.79
F01	Filter Atmospheric	55.00	1.10	56.00	42.00	2.00	0.00	0.00	0.00	0.35	63.58
SC01	Column Atmospheric	55.00	1.10	56.00	42.00	2.00	0.00	0.00	0.00	0.35	63.58
E01	Heat Exchanger S&T	40.00	1.10	56.00	43.97	0.03	0.00	0.00	0.00	0.35	62.46
S01	Separator Atmospheric	5.00	1.10	56.00	43.97	0.03	0.00	0.00	0.00	0.35	62.46
F02	Filter Atmospheric	5.00	1.10	56.00	43.97	0.03	0.00	0.00	0.00	0.35	62.46
C01	Compressor Unspecified	5.00	1.10	56.00	44.00	0.00	0.00	0.00	0.00	0.35	62.30
M01	Vessel Others Pressurized	302.00	20.00	56.00	44.00	0.00	0.00	0.00	0.00	0.35	62.30
L01	Pipeline	75	18.00	97.00	3.00	0.00	0.00	0.00	0.00	0.20	35.82
T01	Tank Pressurized	25.00	18.00	97.00	3.00	0.00	0.00	0.00	0.00	0.20	8596.80
E02	Heat Exchanger S&T	25.00	18.00	97.00	3.00	0.00	0.00	0.00	0.00	0.20	35.82
E02*	Heat Exchanger S&T	833.00	1.10	4.70	5.03	0.00	9.47	9.48	71.28	6.68	1166.22
FU01	Furnaces/Boilers	400.00	1.10	97.00	3.00	0.00	0.00	0.00	0.00	0.20	35.82
FU01*	Furnaces/Boilers	55.00	1.10	5.00	0.15	0.00	0.00	19.92	74.94	6.48	1166.22

* to be considered for physical explosions since it takes into account all the input streams (also the not hazardous ones) to the equipment.

Table S2. Details of the nodes of the hydrogen-based value chain.

NODE	DESCRIPTION	T	P	H_2O	H_2	O_2	N_2	FLOW RATE	INVENTORY
		°C	bar	wt%	wt%	wt%	wt%	kg/s	kg
EL01-1 – EL01-12	Electrolyzer	88.00	30.00	2.08	10.74	87.18	0.00	0.00	9.29
S01-1 – S01-12	Separator (pressurized)	88.00	30.00	10.82	85.06	4.12	0.00	0.01	1.17
S02-1 – S02-12	Separator (pressurized)	88.00	30.00	0.91	0.02	99.07	0.00	0.05	8.12
R01-1 – R01-12	Reactor (tubular)	88.00	30.00	10.82	85.06	4.12	0.00	0.01	1.19
E01-1 – E01-12	Heat Exchanger S&T	88.00	30.00	14.28	85.72	0.00	0.00	0.01	1.17
S03-1 – S03-12	Separator (pressurized)	40.00	30.00	2.22	97.78	0.00	0.00	0.01	1.03
C01	Compressor (unspecified)	40.00	30.00	2.22	97.78	0.00	0.00	0.07	12.31
E02	Heat Exchanger S&T	107.10	50.00	2.22	97.78	0.00	0.00	0.07	12.31
E02*	Heat Exchanger S&T	112.70	50.00	2.22	97.78	0.00	0.00	0.14	24.62
T01	Tank (pressurized)	25.00	50.00	2.22	97.78	0.00	0.00	0.07	2985.00
FU01	Furnace/Boiler	112.70	1.10	2.22	97.78	0.00	0.00	0.07	12.31
FU01*	Furnace/Boiler	26.07	1.10	0.00	0.00	0.23	0.77	6.35	1143.00

* to be considered for physical explosions since it takes into account all the input streams (also the not hazardous ones) to the equipment.

Nomenclature

CH_4	Methane
CO_2	Carbon dioxide
H_2	Hydrogen
H_2O	Water
H_2S	Hydrogen Sulfide
N_2	Nitrogen
O_2	Oxygen
P	Pressure
PFD	Process flow diagram
T	Temperature