Supporting Information

Table S1. Heat and material balance for basic chlorination process

Material Streams											
		BZ In	Cl2 In	Cl2 Out	HCl	Liquid	Upper	Bottom	Benzene to Reactor	Chlorobenzene	Dichlorobenzene
Vapour Fraction		0,0000	0,0000	0,0000	1,0000	0,0000	1,0000	0,0000	1,0000	0,0000	0,0000
Temperature	C	30,00	-50,00	-20,00	25,00	25,00	103,3	175,0	103,3	167,0	212,1
Pressure	kPa	240,0	240,0	240,0	240,0	240,0	240,0	240,0	240,0	240,0	240,0
Molar Flow	kgmole/h	11,52	14,10	14,10	14,41	17,19	5,929	11,26	5,974	8,481	2,779
Mass Flow	kg/h	900,0	1000	1000	540,1	1781	417,7	1363	420,9	955,2	407,9
Liquid Volume Flow	m3/h	1,020	0,6405	0,6405	0,6185	1,663	0,4740	1,189	0,4776	0,8634	0,3260
Heat Flow	kJ/h	5,850e+005	-3,278e+005	-3,021e+005	-1,282e+006	1,629e+005	3,358e+005	3,168e+005	3,384e+005	2,944e+005	3,118e+004

Compositions									
	BZ In	Cl2 In	Cl2 Out	HCl	Liquid	Upper	Bottom	Benzene to Reactor	Chlorobenzene	Dichlorobenzene
Comp Mole Frac (14-Cl-BZ)	0,0000	0,0000	0,0000	0,0002	0,1624	0,0000	0,2480	0,0000	0,0035	0,9941
Comp Mole Frac (Cl-BZ)	0,0000	0,0000	0,0000	0,0039	0,4923	0,0010	0,7510	0,0010	0,9952	0,0059
Comp Mole Frac (Cl2)	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
Comp Mole Frac (Benzene)	1,0000	0,0000	0,0000	0,0167	0,2816	0,8144	0,0010	0,8145	0,0013	0,0000
Comp Mole Frac (HCl)	0,0000	0,0000	0,0000	0,9792	0,0637	0,1846	0,0000	0,1845	0,0000	0,0000
Comp Mole Frac (H2O)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000

Energy Streams							
		QR-101	QC-101	Q-R101	QC-102	QR-102	QE-101
Heat Flow	kJ/h	6,645e+005	1,748e+005	-1,740e+006	5,594e+007	5,596e+007	2,571e+004

Table S2. Heat and material balance for chlorination process after process modification

Material Streams								
		BZ In	Cl2 In	Cl2 Out	Vapor	Liquid	Upper	Bottom
Vapour Fraction		0,0000	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000
Temperature	C	30,00	-50,00	-20,00	25,00	25,00	-24,28	137,5
Pressure	kPa	100,0	100,0	100,0	100,0	100,0	100,0	100,0
Molar Flow	kgmole/h	11,52	14,10	14,10	14,82	16,53	5,026	11,51
Mass Flow	kg/h	900,0	1000	1000	575,4	1780	374,8	1385
Liquid Volume Flow	m3/h	1,020	0,6405	0,6405	0,6561	1,637	0,4250	1,212
Heat Flow	kJ/h	5,849e+005	-3,279e+005	-2,272e+004	-1,249e+006	2,307e+005	1,587e+005	2,525e+005
		Benzene to Reactor	Chlorobenzene	Dichlorobenzene	Bottom-1	HCl	Bottom-Benzene	
Vapour Fraction		0,0180	0,0000	0,0000	0,0000	1,0000	0,0180	
Temperature	C	-10,73	131,2	173,0	83,28	-50,68	-10,76	
Pressure	kPa	100,0	100,0	100,0	100,0	100,0	100,0	
Molar Flow	kgmole/h	5,726	8,917	2,591	0,6998	14,12	5,726	
Mass Flow	kg/h	434,9	1004	380,3	60,07	515,3	434,9	
Liquid Volume Flow	m3/h	0,4890	0,9078	0,3039	6,403e-002	0,5921	0,4890	
Heat Flow	kJ/h	1,931e+005	2,526e+005	8112	3,440e+004	-1,334e+006	1,931e+005	

Compositions							
	BZ In	Cl2 In	Cl2 Out	Vapor	Liquid	Upper	Bottom
Comp Mole Frac (14-Cl-BZ)	0,0000	0,0000	0,0000	0,0005	0,1577	0,0000	0,2265
Comp Mole Frac (Cl-BZ)	0,0000	0,0000	0,0000	0,0097	0,5380	0,0010	0,7725
Comp Mole Frac (Cl2)	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000	0,0000
Comp Mole Frac (Benzene)	1,0000	0,0000	0,0000	0,0380	0,2784	0,9135	0,0010
Comp Mole Frac (HCl)	0,0000	0,0000	0,0000	0,9519	0,0260	0,0855	0,0000
Comp Mole Frac (H2O)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
	Benzene to Reactor	Chlorobenzene	Dichlorobenzene	Bottom-1	HCl	Bottom-Benzene	
Comp Mole Frac (14-Cl-BZ)	0,0012	0,0035	0,9941	0,0102	0,0000	0,0012	
Comp Mole Frac (Cl-BZ)	0,0259	0,9952	0,0059	0,2050	0,0000	0,0259	
Comp Mole Frac (Cl2)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	
Comp Mole Frac (Benzene)	0,8976	0,0013	0,0000	0,7838	0,0010	0,8976	
Comp Mole Frac (HCl)	0,0752	0,0000	0,0000	0,0010	0,9990	0,0752	
Comp Mole Frac (H2O)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	

Energy Streams									
		QR-101	QC-101	Q-R101	QC-102	QR-102	QE-101	QC-103	QR-103
Heat Flow	kJ/h	5,240e+005	3,436e+005	-1,774e+006	1,391e+006	1,399e+006	3,051e+005	5,729e+004	6816