# Hydrogen fluoride

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LIFE CYCLE INVENTORY SUMMARY August 8, 2008

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## Chemistry

Primary reaction:
$CaF_2 + H_2SO_4 \qquad 2HF + CaSO_4 \qquad (1)$ Calcium difluoride + sulfuric acid hydrogen fluoride + calcium sulfate
Side reactions: (type of side rxns)
$SiO_2 + 4HF$ $SiF_4 + 2H_2O$ (2) Silicon dioxide + bydrogen fluoride - silicon tetrafluoride + water
Silicon tetrafluoride + hydrogen fluoride - products (3)
$\frac{1}{\operatorname{Net}(2) + (3)} \qquad \qquad$
$CaCO_3 + H_2SO_4$ $CaSO_4 + CO_2 + H_2O$ (5) Notes: Additional reactions on a small amount of sulfur, aluminum oxide, and iron are not considered in this GTG.

#### **Process Summary**

#### Literature

Virtually all hydrogen fluoride made industrially is from fluorspar. When fluorspar is mined, it is 50% to 90% CaF<sub>2</sub> (Rogers & Muller, 1963; Faith, Keyes, and Clark, 1965). After beneficiation, the upgraded 'acid-grade' fluorspar is 97% (Kirk-Othmer, 2003) 98% (Faith, Keyes, and Clark, 1965) or 98 to 99% (Ullmann's, 2002) calcium difluoride. Hydrogen fluoride is available as an anhydrous liquid or as a 70% aqueous solution, and most is sold in anhydrous form (CEH, 2005). Because HF is formed after reaction in nearly anhydrous form, it is typically refined to near purity (99.98%, Rogers and Muller, 1963) before being diluted as needed.

After beneficiation, the acid grade fluorspar contains 10% moisture (Rogers and Muller, 1963). This material is milled to 170 mesh and dried to less than 0.03% moisture (Rogers and Muller, 1963). Primary impurities are given in Table 1. The silicon dioxide results in a loss of sulfuric acid and hydrogen fluoride. The calcium carbonate results in a loss of sulfuric acid.

	Ullmann's (2002)	Kirk-Othmer (2003)	Rogers and Muller	Faith, Keyes, and Clark	Used in this GTG LCI
				(1965)	report
SiO <sub>2</sub>	1% max	0.7%		1%	1 %
S	0.05% max	0.02%		0.03%	0%
CaCO <sub>3</sub>	1% max	1%			1 %
$Al_2O_3 + Fe_2O_3$	1.5% max				
H <sub>2</sub> O	0.1% max			0.1%	

Table 1. Impurities by weight % in acid-grade fluorspar

Input requirements per kg of HF produced are given in Table 2.

Table 2	Input feed	requirement	s for vield	l calculations	kg feed	/ kø HF
14010 2.	input iccu	requirement	s for yrere	i calculations.	, ng iccu /	Kg III

	$H_2SO_4$	Fluorspar	Comments
Faith, Keyes, and	2.85 (100%)	2.25 (98%)	85-95% yield
Clark (1965)			
CEH (2005)	3 (100%)	2.2	Yield is 85-95%
			from Fluorspar
Kirk-Othmer			Generally, yields
			are > 90% from
			both H <sub>2</sub> SO <sub>4</sub> and
			fluorspar.
Used in this GTG	$2.59 H_2 SO_4 +$	2135 (93% yield)	
report	0.066 SO <sub>3</sub> (92%		
-	yield)		

Faith, Keyes, and Clark (1965) and Rogers and Muller (1963) each give process flow diagrams for HF manufacture. We base our model and that given by Faith, Keyes, and Clark (1965), which is a simplified version of that shown by Rogers and Muller (1963).

The powdered fluorspar is input to a rotating kiln reactor (Kirk-Othmer, 2003), where it is reacted with sulfuric acid. The reactor operates at about 200 oC (Kirk-Othmer, 2003), 100-300 oC (Ullmann's 2002), 250-300 oC (Faith, Keyes, and Clark, 1965). We use a temperature of 250oC in this GTG LCI report. The reaction is endothermic. Ullmann's (2002) gives a heat of reaction of 2,500 kJ per kg HF at 160 oC, and Kirk-Othmer (2003) gives 1400 kJ/kg HF. Side reactions are slightly exothermic, but the heat released is less than 10% of the endothermic heat requirements Ullmann's (2002). We calculate a heat of

reaction at 25 oC of 1500 kJ/kg HF formed including side reactions. The total energy required in the reactor including heating the inputs from 25 oC is 4,200 kJ/kg HF produced.

One difficulty in HF manufacture is keeping the reactor contents well-mixed and transferring heat. During reaction the reactor contents tend to become pasty and corrosive. In the past, these issues limited reactor size and materials. Current reactor technologies allow large reactors to be made from carbon steel (Kirk-Othmer, 2003). We use a standard value for mixing energy (50 MJ/metric ton solids processed).

Several reactor systems are discussed in Ullmann's (2002). In addition to a simple rotary furnace, some operations include a premixer, a prereactor, recycle, or some combination of these. We show a simple reactor. The gas product contains HF, entrained fluorite, heavy impurities such as water and sulfuric acid, and light impurities, such as silicon tetrafluoride, carbon dioxide and sulfur dioxide. Faith, Keyes, and Clark (1965) state that sulfuric acid is fed at 1.1 to 1.3 times the stoichiometric requirement. Rogers and Muller (1963) states that many plants use 1.1 to 1.15 times the stoichiometric requirement, but that their process allows much lower amounts or even stoichiometric amounts of sulfuric acid. Our process feeds 1.08 times stoichiometric amounts to the reactor or a 91% per pass conversion. However, most of the sulfuric acid is recovered and recycled, so that the overall conversion (based on sulfuric and SO<sub>3</sub> fed to the process) of 97%.

On cooling the reactor vapor stream, the sulfur dioxide forms sulfur, which can be removed with cyclones (Ullmanns, 2002). Additionally, some sulfuric acid may be condensed in an externally cooled heat exchanger or the gas can go through a sulfuric acid scrubber. We show condensation of some sulfuric acid and 90% of the water in a precooler and a return to the reactor. Water formed in the reaction is consumed with a portion of oleum (SO3) in the sulfuric acid feed. We show this reaction prior to the reactor.

After the precooler, the vapor is then refrigerated to condense a crude HF stream. Vapor that is not condensed with the HF product stream is fed through a sulfuric acid scrubber to recover HF. The remaining vapor, containing  $CO_2$ , silicon tetrafluoride and some HF is fed to a water scrubber, the silicon tetrafluoride is converted to a salable fluorosilicic acid ( $H_2SiF_6$ ). The HF entering the scrubber is in slight excess of 2 moles per mole of silicon tetrafluoride. This is enough for conversion and leaves a small amount of HF in the fluorosilicic acid (Rogers and Muller, 1963).

The HF is purified by distillation (Kirk-Othmer, 2003; Ullmann's, 2002; Faith, Keyes, and Clark, 1965; Rogers and Muller, 1963). Faith, Keyes, and Clark (1965) states that HF is increased in purity from 98.5% to 99.9% in the distillation by removal of water, sulfuric acid, and sulfur dioxide. Ullmann's states that the distillation generally requires two columns. U.S. 4,954,330 states that distillation is used to remove impurities such as  $SO_2$ ,  $H_2SO_4$ , water, and  $SiF_4$ , and fluorosulfonic acid. We show two columns, in the sequence given by Rogers and Muller (1963). The first removes lower boilers, and the second distills the HF product from any heavier contaminants.

Calcium sulfate forms as a by-product of the reaction in large quantities. This calcium sulfate can be used in cement or other applications in building mining and road construction. However, these applications have only been used in Germany and Japan (Ullmann's, 2002). The calcium sulfate by-product is generally not used in the U.S. (Ullmann's, 2002). Kirk-Othmer (2003) also states that calcium sulfate is generally not recovered in this process in the U.S. because natural gypsum is plentiful. Rogers and Muller state that calcium sulfate is generally not recovered; however, they mention that it is recoverable for use as a building material from their process. We show this stream as a waste. It should be noted that this decision has a large impact on the allocated LCI, as the total liquid products are 1000 kg/hr HF and 46 kg/hr  $H_2SiF_6$ . The calcium sulfate stream is 3,680 kg/hr.

The fluorspar input to the process is 'acid grade,' thus, it has been beneficiated to 97-98% CaF<sub>2</sub>. In addition, milling and drying is required prior to use in HF manufacture. We do not have a mining report specific to fluorspar. Thus, we currently use generic underground mining LCI from BUWAL. We assume that this is for the acid grade product with 10% moisture. We show drying as a separate sequence of steps in this report, and include the energy requirements in the LCI.

#### LCI design

Input fluorspar is milled and dried to 0.03% moisture content (shown separately from the rest of the process). This is fed to the reactor in stream 5. Sulfuric acid with a small portion of SO<sub>3</sub> is fed to a scrubber to capture HF and H<sub>2</sub>SO<sub>4</sub> vapors recycled from the chilled crude HF stream. The vapors are fed to a water scrubber for recovery of fluorosilicic acid, which is sold as a by-product. The liquid from the sulfuric acid scrubber is combined with another recycle stream (largely water and sulfuric acid), where the water (formed in reaction) combines with the SO<sub>3</sub> in the oleum to form sulfuric acid prior to the reactor.

The reactor, operating at 250 oC is heated with Dowtherm. The product stream leaves as a vapor, and is pre-cooled. A liquid / gas separator is used to recover most of the sulfuric acid and water for recycle. A refrigeration system is used to cool the crude HF to 10 oC. Some remaining vapor is sent to the sulfuric acid scrubber mentioned previously. The liquid (crude HF) is refined in two distillation columns. In the first, a small amount of impurities is recovered, and hence the energy requirements are minimal. In the second, HF is distilled from heavier components, including water. This separation is fairly easy considering the large boiling point difference. In the second column, we estimate the relative volatility from data in Kirk-Othmer (2003).

#### **Calculation notes:**

Fluorspar has a Bond Work index of 9.76 kWhr/metric ton. Mesh 170 corresponds to 88 microns. Thus, the energy of grinding can be estimated as 9.76\*(10/sqrt(88 microns)) = 10.4 kWhr/metric ton or 88 MJ/1000 kg of HF produced.

CEH (2005) Chemical Economics Handbook. Fluorspar and Inorganic Fluorine Compounds (R. Will and Y. Ishikawa, report authors).

Faith W.L., D.B. Keyes, and R.L. Clark (1965). Industrial Chemicals, Wiley & Sons, New York, 3<sup>rd</sup> ed. page 462.

Kirk-Othmer (2003) Kirk Othmer Encyclopedia of Chemical Technology. Fluorine Compounds, Inorganic, Hydrogen (R. Smith, article author).

Ullmann's (2002) Ullmann's Encyclopedia of Industrial Chemistry. Fluroine Compounds, Inorganic (Jean Aigueperse, Paul Mollard, Didier Devilliers, Marius Chemla, Robert Faron, René Romano, Jean Pierre Cuer, article authors).

Rogers, W.R. and Muller, K. (1963). Hydrofluoric acid manufacture. Chemical Engineering Progress, Vol 59, No 5. pp. 85-88.

#### **Critical parameters**

Conversion / Yield information from both reactors										
		Conversion of or Yield from H 2SO 4	Conversion of or Yield from CaF_2							
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	96.7 (includes SO_3 input)	98.2							
Total per pass conversion in reactor 1: (% of reactant entering the reactor that reacts)	From mass balance	90.6	98.2							
Total yield of reactor 1: (% yield HF produced in the reactor based on reactant input to process)	From mass balance	96.5	97.3							
Total yield of Process:	From mass balance	92 (includes SO_3)	93							

(% yield produced by the overall		
process based on reactant input to		
process)		
Notes:		

Product purity		
	HF	Comments
Used here	99.98	
LiteratureSource	99.98	Rogers and Muller (1963)

				Inpu	ts								
Input UID	Input Name	Input Flow	Input purity	Units	Comments								
7446-11-9	Sulfur trioxide	65.8		[kg/hr]									
14542-23- 5	Fluorspar												
7664-93-9	Sulfuric acid	2588		[kg/hr]									
	Total	4787		[kg/hr]									
Non-reacting inputs													
UID	Name	Flow	Purity	Units	Comments								
7732-18-5	Water	105		[kg/hr]									
	Total	105		[kg/hr]									
	Ancillary inputs												
UID	Name	Flow	Purity	Units	Comments								
No ancilla	ry inputs												
		i		Produ	cts								
Product UID	Product Name	Product Flow	Purity	Units	Comments								
16961-83- 4	Fluorosilicic acid	46.1	98.9	[kg/hr]	This is flow of H2SiF6. Impuritiy is HF. Stream also contains 105 kg water, considered a benign output.								
7664-39-3	Hydrogen fluoride	1000	100.0	[kg/hr]									
	Total	1046		[kg/hr]									
		-	Ве	enign Ou	utflows								
UID	Name	Flow	Purity	Units	Comments								
7732-18-5	Water	107		[kg/hr]	Included 105 kg water in fluorosilicic acid byproduct.								
	Total	107		[kg/hr]									

# Summary of LCI Information

	Chemical Emissions													
Emission UID	Emission Name	Gas Flow	Liquid Flow	Solid Flow	Solvent Flow	Units	Comments							
7664-39-3	Hydrogen fluoride	5.20	11.1	0	0	[kg/hr]								
7783-61-1	silicon tetrafluoride	0.185	3.66	0	0	[kg/hr]								
7446-11-9	Sulfur trioxide	1.32	0	0	0	[kg/hr]								
7778-18-9	Calcium sulfate	0	0	3608	0	[kg/hr]								

124-38-9	Carbon dioxide	9.43 0		0	0	[kg/hr]	
7664-93-9	Sulfuric acid	0	32.3	36.1	0	[kg/hr]	
7789-75-5	Calcium Difluoride	0 0		38.0	0	[kg/hr]	
Totals		16.1	47.1	3682	0	[kg/hr]	
	-		Ν	lass Bala	nce		-
Total inputs		4892					
Total outflow	WS	4899					
Net input		-6.44					
				Energy u	se		
Energy type		Amount Comment					
electricity					616	[MJ/hr]	
heating stear	m				2784	[MJ/hr]	
dowtherm					2870	[MJ/hr]	
Net input re	quirement				6270	[MJ/hr]	Net of energies input to system
cooling wate	er						
potential rec	overy				-297	[MJ/hr]	
Net energy				5973	[MJ/hr]	Net input requirement - potential recovery	

#### **Process Diagram Interpretation Sheet**

- 1) As much as possible, standard symbols are used for all unit processes.
- 2) Only overall input and output chemicals are labeled on these diagrams. All intermediate information is given on the attached Process Mass Balance sheet
- 3) The physical state of most streams is shown (gas, g; liquid, l; solid, s)
- 4) The process numbering is as follows,
  - generally numbers progress from the start to the end of the process
  - numbers are used for process streams
  - C i , i = 1,..n are used for all cooling non-contact streams
  - S j, j = 1,...n are used for all steam heating non-contact streams
- 5) Recycle streams are shown with dotted lines

For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

#### **Process Diagram or Boundary of LCI**

Steam enters the process as a gas at 207 °C and leaves as a liquid at 207 °C. Cooling water enters at 20 °C and leaves at 50 °C. Unless otherwise indicated, all processes are at 1 atm and 25°C.



\*Mx 1 combines oleum (a portion of SO3, which reacts with water to form H2SO4 prior to the reactor



Evan Griffing

## **Mass Balance of Chemicals in Each Process Stream**

All flow rates are given in kg / hr Physical state of chemical losses:

Gas Liquid Solid

	Com	Streams	Те	ΓP	P	Total	Wa	Sulf	FI	Ca	Car	Su	silic	Flu	Hy	Cal	Sili	Cal	s	Water
	ment		m		h	Flow	ter	uric	u	lci	bon	lfur	on	or	dro	ciu	са	ciu	t	
	S		р		a			acid	or	um	diox	trio	tetr	osi	ge	m		m	е	
					S				S	Sul	ide	xid	aflu	lici	n	Difl		car	a	
			1		e				p			e	ona		rid	ide		00 nat	m	
									ai				C	d	e	lue		e		
Input			1 25.	01.0	01	2654		2588	0	0	0	65.8	0	0	0					
			2 25.	0 1.0	01	2654	0	2588				65.8								
		Stream 12:Recycle input				72.6					9.26		33.3		30.0					
		Stream 12:Recycle calcu	lated			72.7	0	0	0	0	9.39	0	33.3	0	30.0	0	0	0		
		Stream 12:Recycle residue				-0.110	0	0	0	0	-0.127	0	0.0171	0	0	0	0	0		
		:	3 25.	0 1.0	01	2670	0	2588	0	0		65.8			16.7	0	0	0		
		Stream 9:Recycle input				215	14.8	200												
		Stream 9:Recycle calcula	ated			215	15.0	200	0	0	0	0	0	0	0	0	0	0		
		Stream 9:Recycle residue				0.191	-0.177	0.368	0	0	0	0	0	0	0	0	0	0		
		4:	a 25.	0 1.0	01	2885	14.8	2788	0	0	0	65.8	0	0	16.7	0	0	0		
		water / SO3 reaction coefficients	•			-1.00	-1.00	1.00				-1.00								
		water / SO3 reaction kg/hr				0	-14.8	80.6				-65.8								
		water / SO3 reaction kgn	nol/hr			-0.822	-0.822	0.822				-0.82 2								
			4 25.	0 1.0	01	2885	0	2868	0	0	0	0	0	0	16.7	0	0	0		
Input			5 25.	0 1.0	0 s	2134			2134											
		5 component	s 25.	0 1.0	0 s	2134	0									2091	21.3	21.3		
R1	2053	kg	Calc Diflu	ium oride	9	is converted in rxn 1 ( 98.2 % of	50.0	kJ/gmol												
						linput)														
	21.3	kg	Silic	a		is lost in rxn 2	1000	kJ/kg												
12		1	Evan (	Griffi	ng				August	8,200	8									<u>.</u>

	Com	Streams	Те	Р	P	Total	Wa	Sulf	FI	Са	Car	Su	silic	Flu	Hy	Cal	Sili	Cal	S	Water
	ment		m		h	Flow	ter	uric	u		bon	lfur	on	or	dro	ciu	са	ciu	t	
	s		p		a			acid	or		diox	trio	tetr	OSI   lici	ge	m Difl		m	e	
									n n	fat	lue		orid		fluo			bo	m	
			1.		1				ar	e			e	aci	rid	ide		nat		
									C.I.				Ű	d	e			e		
	21.3	kg	Calci	um		is lost in														
			carbo	nate		rxn 3													<u> </u>	
		Input to reactor			:	5019	0	2868	0	0	0	0	0	0	16.7	2091	21.3	21.3	<u> </u>	
		R1 Reaction Coefficient 1			:			-1.00		1.00					2.00	-1.00		<u> </u>		
		R1 Conversion 1 [kg/hr]			:	0		-2579		3579					1053	-2053		<u> </u>		
		R1 Conversion 1 [kgmol/hr]			:	26.3		-26.3		26.3					52.6	-26.3				
		R1 Reaction Coefficient 2			:		2.00						1.00		-4.00		-1.00			
		R1 Conversion 2 [kg/hr]			:		12.8						37.0		-28.4		-21.3			
		R1 Conversion 2 [kgmol/hr]			:	0.356	0.711						0.356		-1.42		-0.356			
		R1 Reaction Coefficient 3			:		1.00	-1.00		1.00	1.00							-1.00		
		R1 Conversion 3 [kg/hr]			:		3.84	-20.9		29.0	9.39							-21.3		
		R1 Conversion 3			:		0.213	-0.213		0.213	0.213							-0.213		
		Flow out of reactor				5019	16.6	268	0	3608	0 30	0	37.0		1041	38.0	0	0	<u> </u>	
		Primary product			:	Hydrogen	10.0	200			0.00		01.0		1011	00.0				
		Tatal as musican				fluoride	45.0	00.7											┝──	
					:		-15.8	96.7	-0			-0	NA	INA	NA		INA 400		┝───	
		Per pass conversion			Ë.		NA	90.6			NA		NA		NA	98.2	100	100	<u> </u>	
		lotal yield from reactor	050	1.00	:	0000		96.5	0	Error					NA	97.3				
Waste		6	250	1.00	S	-3682	0	-36.1	0	-3608	0	0	0	0	0	-38.0	0	0	0	0
	77.9 % HF	7	250	1.00	g	1336	16.6	232	0	0	9.39	0	37.0	0	1041	0	0	0		
		8	25.0	1.00	g	1336	16.6	232	0	0	9.39	0	37.0	0	1041	0	0	0		
		9	25.0	1.00		215	15.0	200												
		10	25.0	1.00	g	1122	1.66	32.5	0	0	9.39	0	37.0	0	1041	0	0	0		
		11	10.0	1.00	g	1122	1.66	32.5	0	0	9.39	0	37.0	0	1041	0	0	0		
		12	10.0	1.00	g	72.7					9.39		33.3		30.0					
		13	25.0	1.00	g	56.0	0	0	0	0	9.39	0	33.3	0	13.3	0	0	0		
Input		14	25.0	1.00		105	105													
		scrubber_rxn_coefficients				-2.00							-1.00	1.00	-2.00					
		scrubber_rxn_kg/hr				0							-33.3	46.1	-12.8					
		scrubber_rxn_kgmol/hr											-0.320	0.320	-0.640					
By-proc	duct	15	25.0	1.00	I	-152	-105	0	0	0	0	0	0	-46.1	-0.507	0	0	0	0	0
Waste		16	25.0	1.00	g	-9.39	0	0	0	0	-9.39	0	0	0	0	0	0	0	0	0
13		ŀ	Evan G	riffin	g				August	8, 200	8									

	Com	Streams	Те	Р	P	Total	Wa	Sulf	FI	Ca	Car	Su	silic	Flu	Hy	Cal	Sili	Cal	S	Water
	ment		m		h	Flow	ter	uric	u	lci	bon	lfur	on	or	dro	ciu	ca	ciu	t	
	S		р		a			acid	or	um	diox	trio	tetr	osi	ge	m		m	е	
					S				S	Sul	Ide	XID	aflu		n fluo	Difl		car	a	
			]		e e				p			e	ona		rid	ide		00 nat	m	
									a				E	d	e	lue		e		
		17	10.0	1.00	1	1049	1.66	32.5	0	0	0	0	3.70	0	1011	0	0	0		
	Feed	18	10.0	1.00	1	1049	1.66	32.5	0	0	0	0	3.70	0	1011	0	0	0		
Di 1		percentage of input in disti	llate		:		0.500	0.500					99.0		0.100					
		percentage of input in bott	oms		:		99.5	99.5					1.00		99.9					
		Boiling Temperature (Tb) [	oC]		:		99.9	340					-86.2		19.5					
Waste	Distillat	19	10.0	1.00	1	-4.84	-8.32	-0.162	0	0	0	0	-3.66	0	-1.01	0	0	0	0	0
-	е						E-03													
	Bottoms	20	10.0	1.00	I	1044	1.66	32.3	0	0	0	0	0.0370	0	1010	0	0	0		
	Feed	21	10.0	1.00	I	1044	1.66	32.3	0	0	0	0	0.0370	0	1010	0	0	0		
Di 2		percentage of input in disti	llate		:		0.500	0.500					99.9		99.0					
		percentage of input in bott	oms		:		99.5	99.5					0.1000		1.00					
		Boiling Temperature (Tb) [	oC]		:		99.9	340					-86.2		19.5					
Main	Distillat	22	19.5	1.00	I	-1000	-8.28	-0.162	0	0	0	0	-0.036	0	-1000	0	0	0	0	0
product	e Dottomo	0.0	10 E	1.00		42.0	E-03	20.0	0	0	0	0	2 705	0	10.1	0	0	0	0	0
vvaste	BOlloms	23	19.0	1.00		-43.9	-1.00	-32.2	0	0	0	0	-3.70E -05	0	-10.1	0	0	0	0	0
		P1	25.0	1.00	s	2371	237		2134											
		P2	25.0	1.00	s	2371	237		2134											
		P3	25.0	1.00	s	2371	237		2134											
		P4	100	1.00	g	236	236													
		P5	100	1.00	s	2134	0.640		2134											
		Product purity (%)				100.0														
		Main product				Hydrogen fluoride														
		Overall Rxn coefficients			Ī			-1.00							2.00	-1.00				
		Total yield of process (fron	n	İ				91.8							NA	Error				
		reactant)																		
Waste		Fugitive Losses (Total)			g	-6.75	0	0	0	0	-0.046 9	-1.32	-0.185	0	-5.20	0	0	0	0	0
		Input Sum				4892	105	2588	2134	0	0	65.8	0	0	0	0	0	0		
		Fugitive Replacement of Reactants				0		0								0				
		Total Input (Input + Fugitiv Replacement)	е	-		4892	105	2588	2134	0	0	65.8	0	0	0	0	0	0		
		Product Sum				1152	105	0.162	0	0	0	0	0.0369	46.1	1000	0	0	0		

	Com	Streams	Те	Р	Ρ	Total	Wa	Sulf	FI	Са	Car	Su	silic	Flu	Ну	Cal	Sili	Cal	S	Water
	ment		m		h	Flow	ter	uric	u	lci	bon	lfur	on	or	dro	ciu	са	ciu	t	
	S		р		а			acid	or	um	diox	trio	tetr	osi	ge	m		m	е	
			[C		s				S	sul	ide	xid	aflu	lici	n	Difl		car	а	
			J		е				р	fat		e	orid	С.	fluo	uor		bo	m	
									ar	e			е	aci	rid	ide		nat		
		Main product flow				1000	0.00	0.100	0	<u> </u>			0.0200	u o	e 1000			e		
		Main product now				1000	8.28E -03	0.162	0	0	0	0	0.0369	0	1000	0	0	0		
		Net Input (in - out, omitting fugitives)	1			-0.191														
Input		C1	20.0	1.00	I	4477														4477
Coolin		C2	50.0	1.00	1	-4477	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>0</u>	-4477
g out																				
Input		C3	20.0	1.00	I	1.05E+04														1.05E+0
Coolin		C4	50.0	1 00	1	-1 05E+0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1 05E+0
a out		<b>U</b> T	00.0	1.00		4		¥		_ ⊻	<u> </u>	_ ⊻	<u> </u>		<u> </u>		_ ⊻			4
Input		C5	20.0	1.00	I	129														129
Coolin		C6	50.0	1.00	1	-129	0	0	0	0	0	0	0	0	0	0	0	0	0	-129
g out																				
Input		C7	20.0	1.00	Ι	1.06E+04														1.06E+0
																				4
Coolin		C8	50.0	1.00	I	-1.06E+0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.06E+0
y out Input		S1	207	1 00	1														11 7	4
Stoom		51	207	1.00	1	11.7	0	0	0	0	0	0	0	0	0	0	0	0	11.7	0
out		52	207	1.00		-11.7	0	0	0	0	0	0	0	0	0	0	0	0	7	0
Input		S3	207	1.00	1	975													975	
Steam		S4	207	1.00	1	-975	0	0	0	0	0	0	0	0	0	0	0	0	-97	0
out																			5	
Input		S5	207	1.00	1	469													469	
Steam		S6	207	1.00		-469	0	_0	0	.0	_0	0_	_0	0	0	_0	0	_0	-46	0
out																			9	

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## **Graph of Cumulative Chemical Losses through Manufacturing Process**

**Cumulative Chemical Loss** 



## **Graph of Cumulative Contaminated Water Use / Emission through Manufacturing Process**

Cumulative Contaminated Water Use



## Graph of Cumulative Non-Contaminated Water Use / Emission through Manufacturing Process



**Cumulative Non-Contamintated Water Use** 

# Energy Input for each Unit Process, Cumulative Energy Requirements, Cooling Requirements (exotherms), and Assumed Heat Recovery from Hot Streams Receiving Cooling

Energy	Input [MJ / batc	h]				Cooling Requirements [MJ / batch]											
Process Diagra m Label	Unit	Energy input [MJ / 1000 kg Product]	Cumulat ive energy [MJ / 1000 kg Product]	To [C] (Us ed to dete rmin e ener gy type )	Energy Type	Proce ss diagr am label	Unit	Energy Loss	Cumula tive cooling water energy	Tef [C] (for reco very effic ienc y)	Recove ry Efficien cy	Energy Recove red	Cumul ative recover ed [MJ / 1000 kg Produc t]				
P1	Pump 1	0.0881	0.0881	/	Е	Hx1	Heat exchanger 1	-661	-661	250	0.450	-297	-297				
R1	Reactor 1	2870	2870	250	D	Ref1	Refrigerator cooling 1	-1546	-661	25	0	0	-297				
MxE1	Mixer electricity 1	184	3054		E	Di1	Distillation condenser	-19.1	-680	10.0	0	0	-297				
Ref1	Refrigerator elect. 1	426	3480	0	E	Di2	Distillation condenser 2	-1563	-2243	18.5	0	0	-297				
P2	Pump 2	6.06E-03	3480		E												
P3	Pump 3	2.44E-04	3480		Е												
Di1	Distillation reboiler 1	19.1	3499	10.0	S												
P4	Pump 4	2.40E-04	3500		E												
Ref2	Refrigerator elect. 2	5.26	3505	0	E												
Di2	Distillation reboiler 2	1585	5090	18.5	S												
Cnv1	Conveyer 1	9.96E-03	5090		E												
na	Ball mill	88.8	5179	0	0												
Dry1	Dryer 1	762	5941	100	S												
	Potential recovery	-297	5644														
	Net energy		5644				Potential recovery:						-297				
	Electricity	616	E	[MJ/hr]							i						
	DowTherm	2870	D	[MJ/hr]													
	Heating steam	2367	S	[MJ/hr]													
	Direct fuel use	0	F	[MJ/hr]													
	Heating natural gas	0	G	[MJ/hr]													
	requirement	5852		[MJ/hr]													
	Cooling water	-2243		[MJ/hr]													
	Cooling refrigeration			[MJ/hr]													

Potential heat	-297	[MJ/hr]					
recovery							
Net energy	5555	[MJ/hr]					

## **Graph of Cumulative Energy Requirements**





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