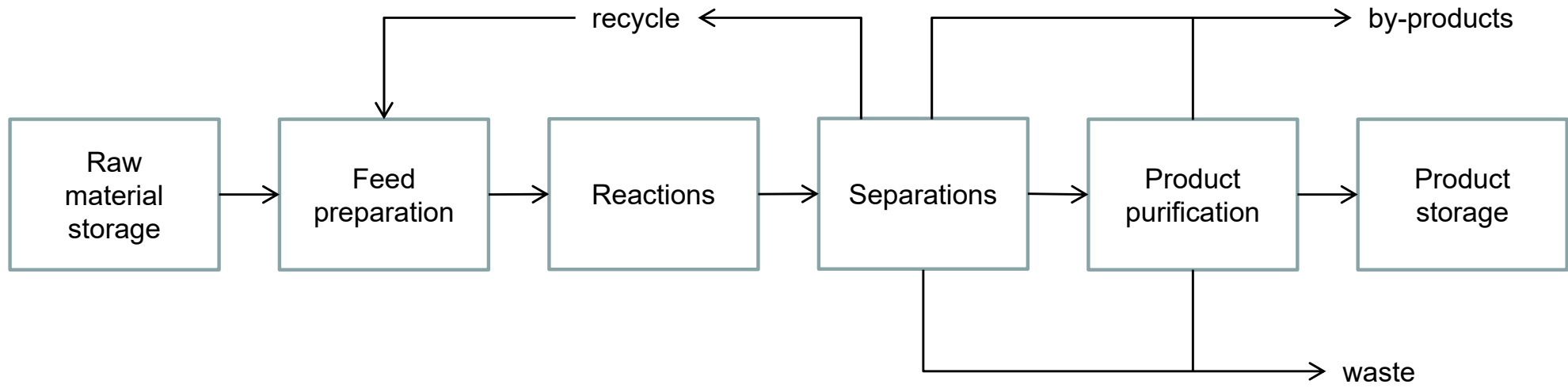


CH402 Chemical Engineering Process Design

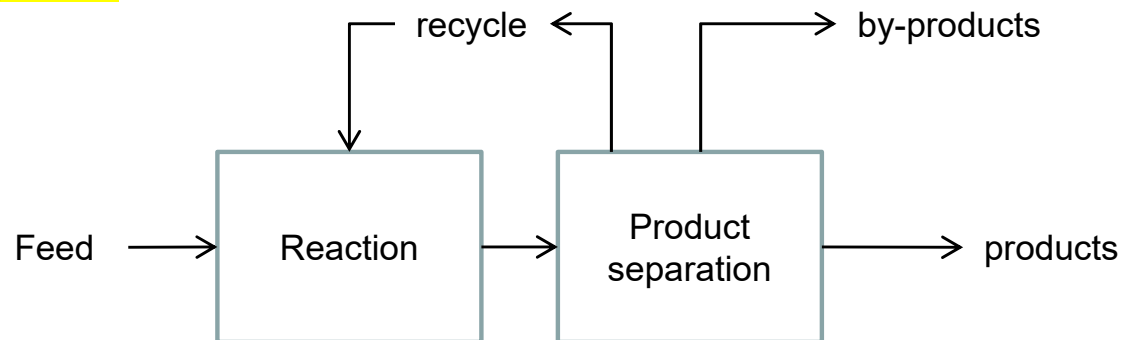
Class Notes L13

Flowsheet Synthesis and I/O Analysis

Block Diagram of (all) Chemical Processes



“Function Diagram”



Q's may or may not be shown

Often simplified to this form.

Case Study - Vinyl Chloride Monomer (VCM) Production

47 million tons/y in 2025 worldwide

57 million tons/y in 2030 (est.) 3.87% growth to 2030

<https://www.mordorintelligence.com/industry-reports/vinyl-chloride-monomer-market>

12 US plants, average capacity is 667,000 t/y

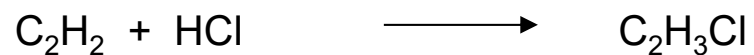
J.A. Cowfer and M.B. Gorenssek, 19 May 2006, Kirk-Othmer Encyclopedia of Chemical Technology,
<https://doi.org/10.1002/0471238961.2209142503152306.a01.pub2>

Known Vinyl Chloride Routes

Next step is a literature search – 5 Routes Identified

Kirk-Othmer, Wikipedia

(CH383)



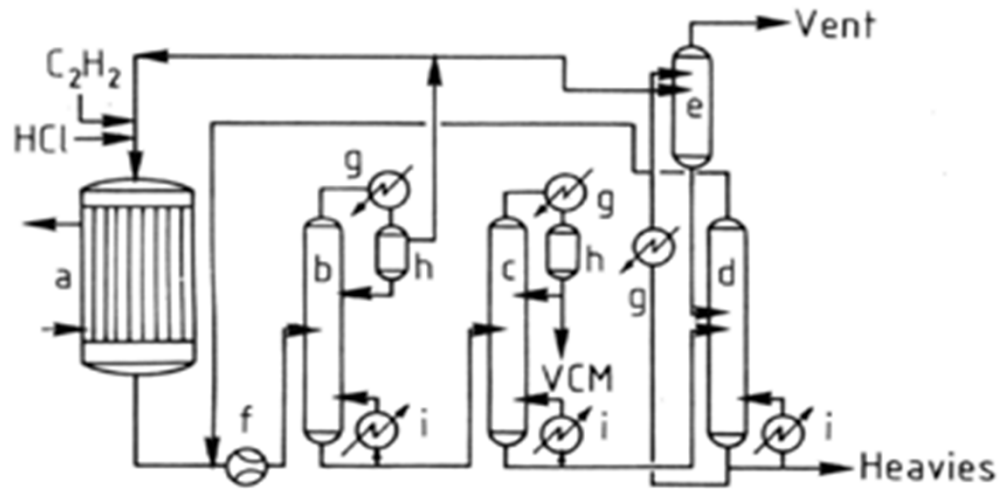
Route 1

direct reaction of acetylene
(acetylene hydrochlorination)

Vinyl Chloride Process Flow Diagram

Ullmann's Encyclopedia of Industrial Chemistry

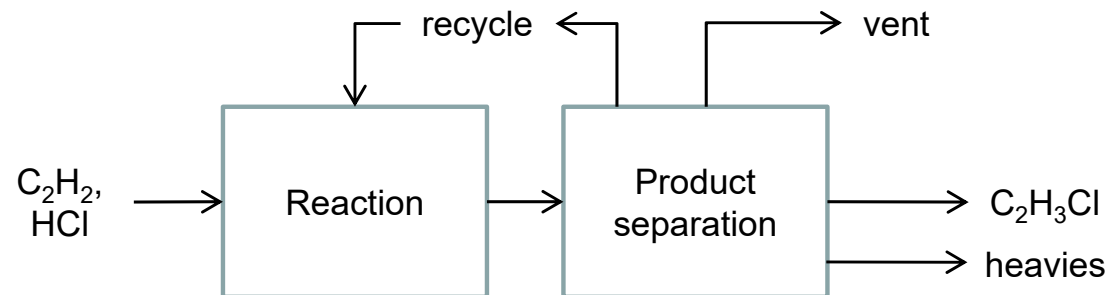
Dreher, L., Beutel, K.K., Myers, J.D., Lübke, T., Krieger, S., & Pottenger, L.H., Chloroethanes and Chloroethylenes. 1-81.



d, #Jhdfwru
 e, #Djkw#Eroxp q
 f, #FP #Eroxp q
 g, #Kdy| #wls shu
 h, #Hqw#z dvk #r z hu
 j, #Erqghqvhu
 k, #Jhix { #uxp
 l, #Jherlhu

Surfhvv#Erz #G ldjudp #SIG ,
 Vp lduw#FKHP FDG

Ixqfwlrq#G ldjudp

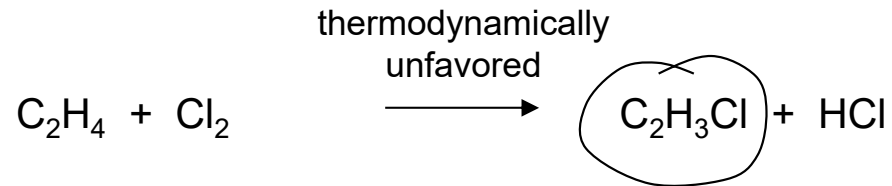


Known Vinyl Chloride Routes

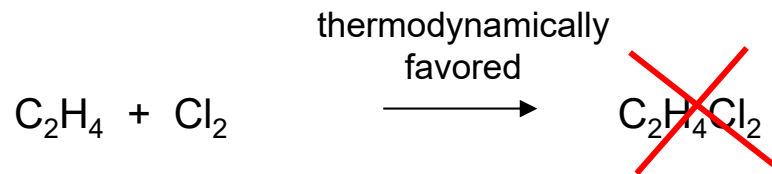
Kirk-Othmer, Wikipedia

Literature Search

(also CH383)



Route 2
direct chlorination of
ethylene (liquid phase)



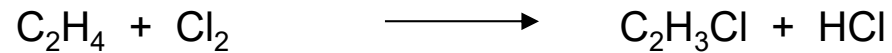
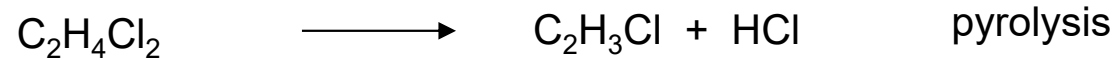
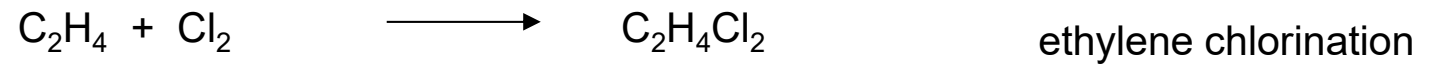
Not the product we want

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

Literature Search

CH383

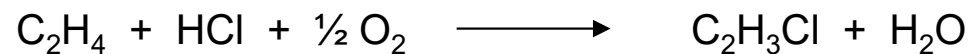
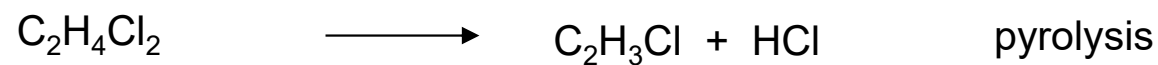


Route 3
direct chlorination + pyrolysis

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

Literature Search



Route 4
oxychlorination + pyrolysis

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

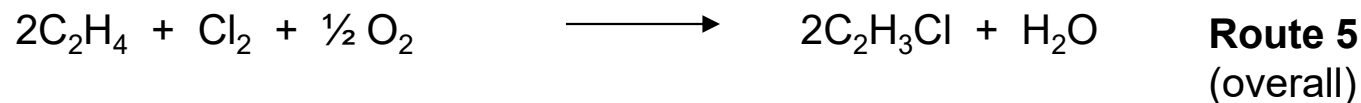
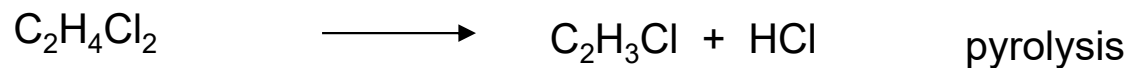
Literature Search



+



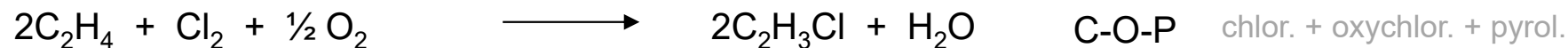
+



Known Vinyl Chloride Routes

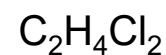
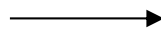
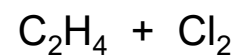
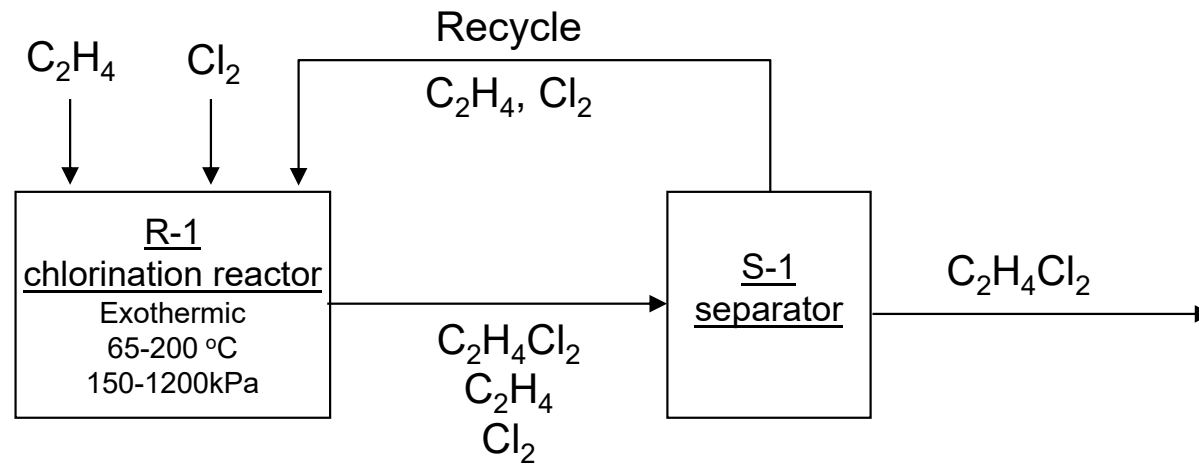
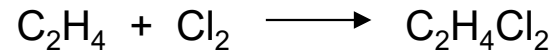
5 processes identified in literature survey

Summary



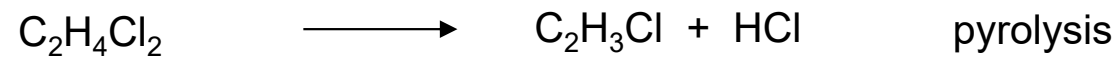
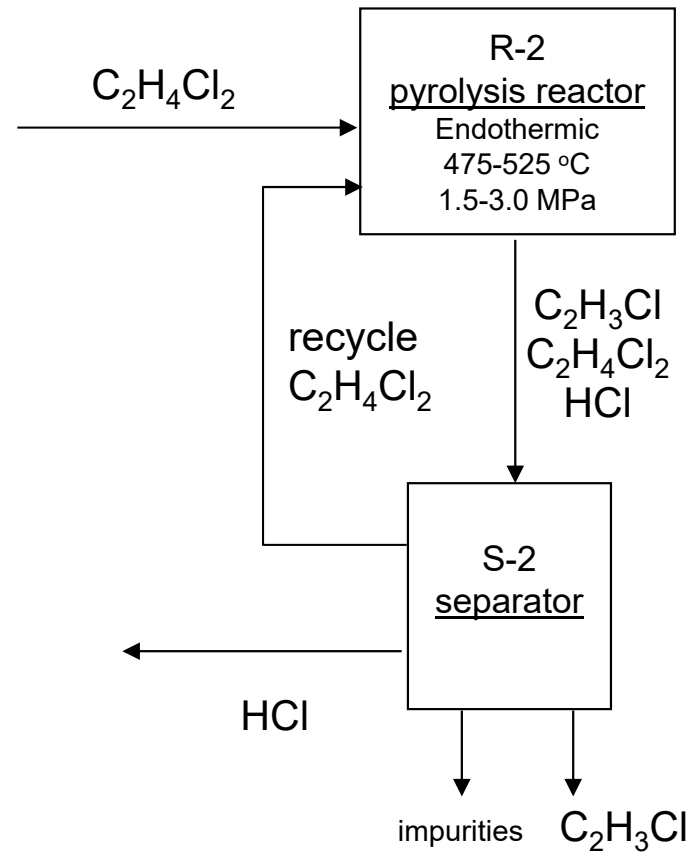
Functions Diagram – C – Direct Chlorination

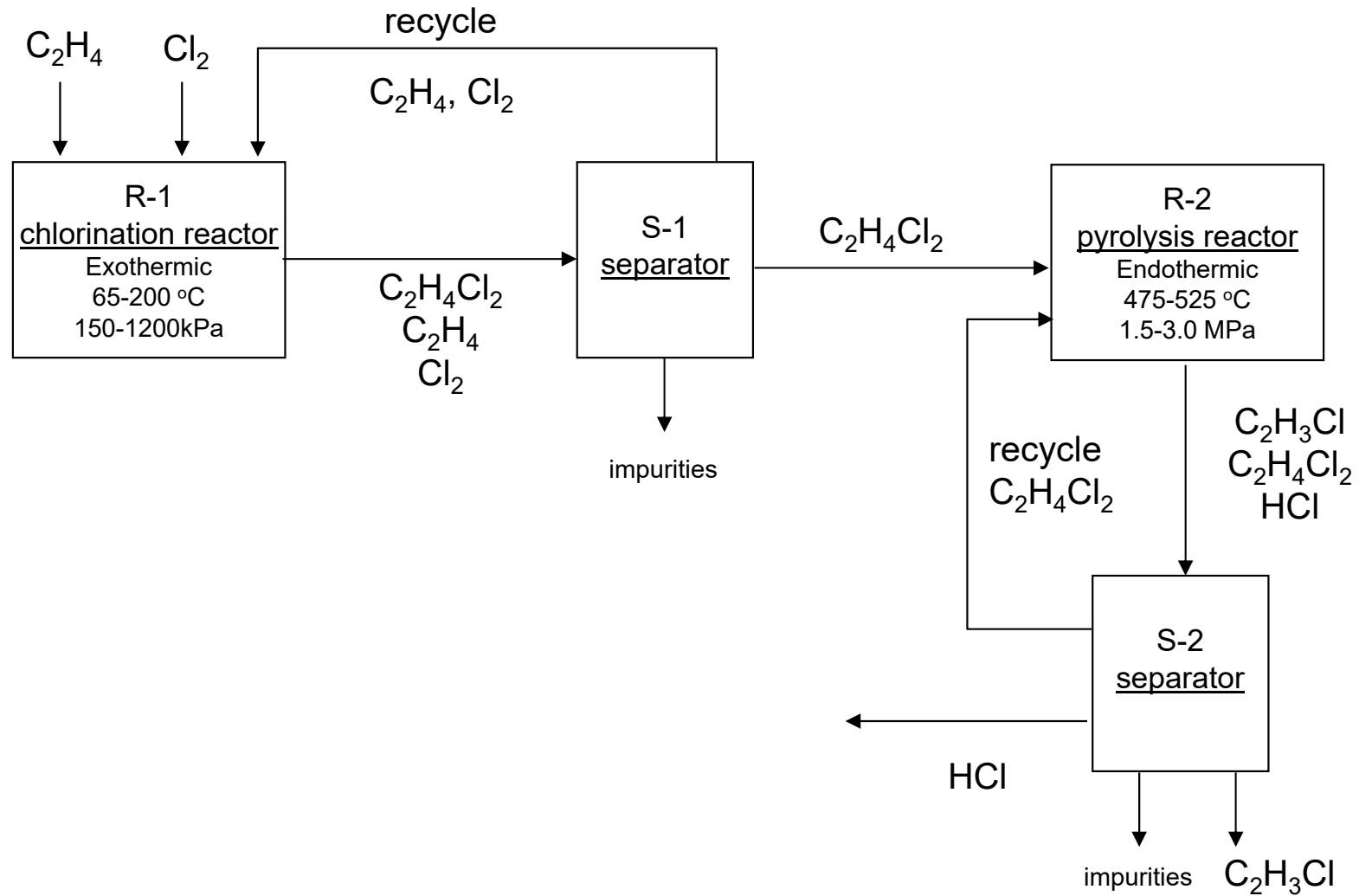
The utility of the functions diagram is that it can be used to build much larger processes.



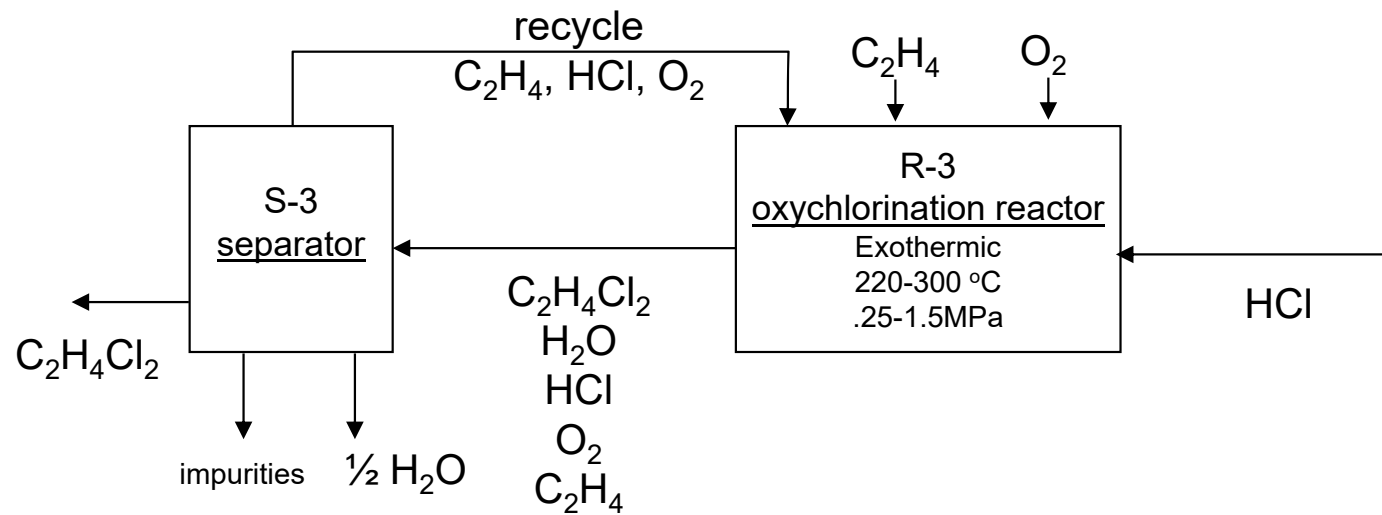
ethylene chlorination

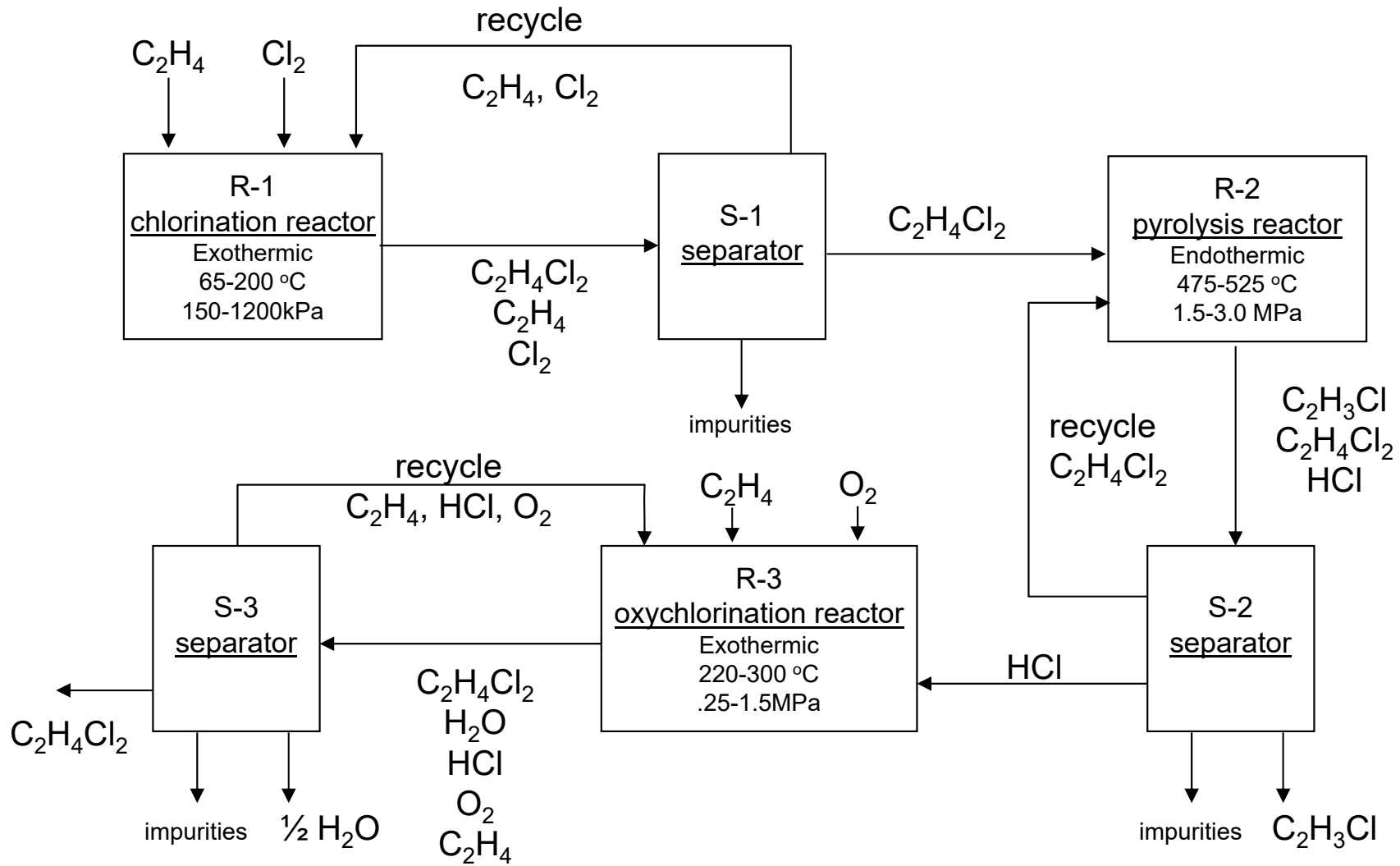
Functions Diagram – Pyrolysis

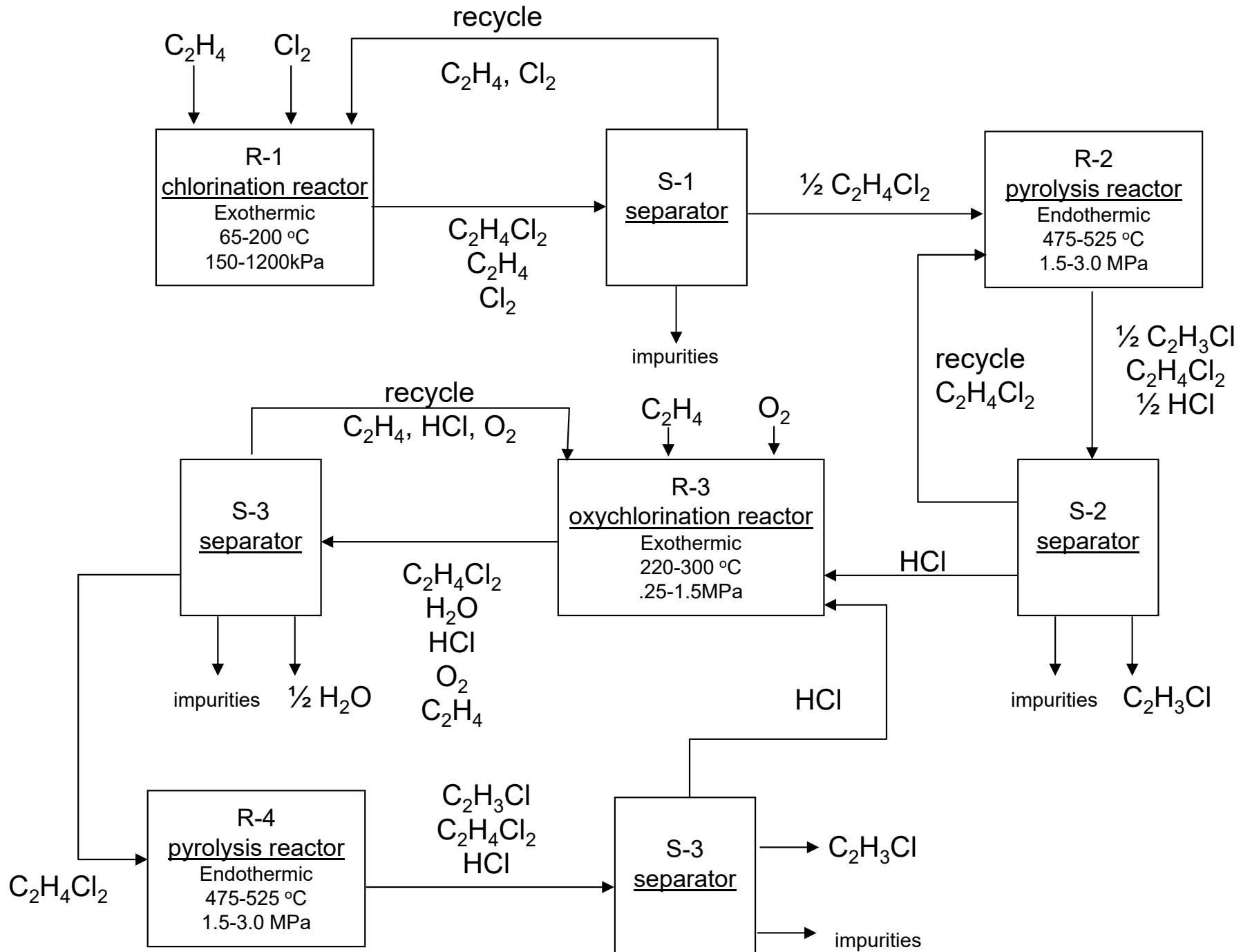


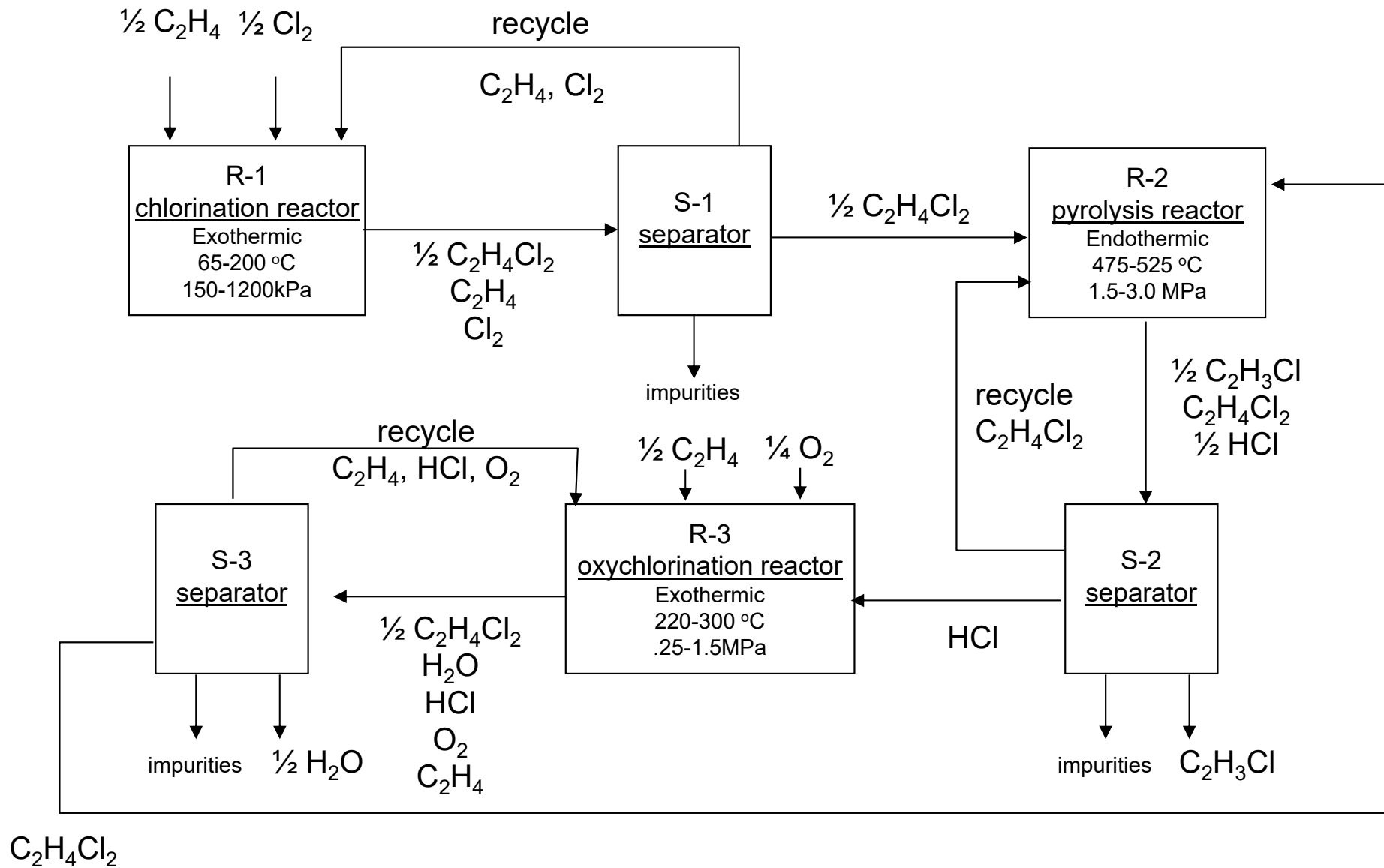


Functions Diagram – Oxychlorination



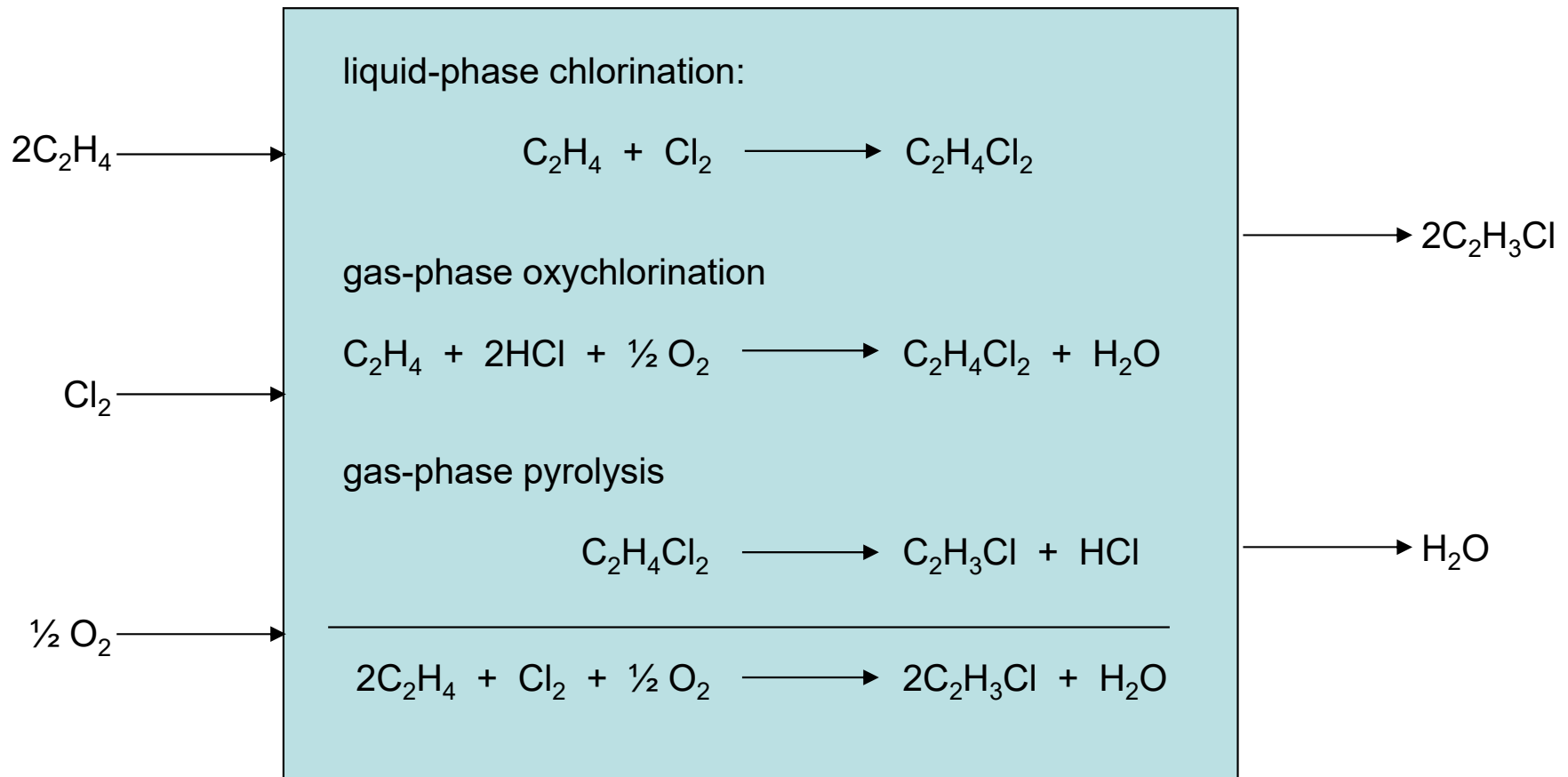






Input/Output Structure - Route 5 - COP

I/O box is frequently left blank



The I/O analysis allows us to assess the overall economics of the process.

Known Vinyl Chloride Routes

5 processes

				Reaction Path
$\text{C}_2\text{H}_2 + \text{HCl}$	\longrightarrow	$\text{C}_2\text{H}_3\text{Cl}$	A	1
$\text{C}_2\text{H}_4 + \text{Cl}_2$	\longrightarrow	$\text{C}_2\text{H}_3\text{Cl} + \text{HCl}$	C	2
$\text{C}_2\text{H}_4 + \text{Cl}_2$	\longrightarrow	$\text{C}_2\text{H}_3\text{Cl} + \text{HCl}$	C-P	3
$\text{C}_2\text{H}_4 + \text{HCl} + \frac{1}{2} \text{O}_2$	\longrightarrow	$\text{C}_2\text{H}_3\text{Cl} + \text{H}_2\text{O}$	O-P	4
$2\text{C}_2\text{H}_4 + \text{Cl}_2 + \frac{1}{2} \text{O}_2$	\longrightarrow	$2\text{C}_2\text{H}_3\text{Cl} + \text{H}_2\text{O}$	C-O-P	5

Economic Analysis is Based on I/O

Measures the economic “driving force”

Example 4-2, page 135

Species	MW, kg/kgmol	Price, \$/kg	Reaction Path, kg/kg VC				
			1	2	3	4	5
Cl ₂	70.9	0.03	---	-1.13	-1.13		-0.57
HCl	36.5	0.22	-0.58	0.58	0.58	-0.58	---
C ₂ H ₂	26.0	1.39	-0.42	---	---	---	---
C ₂ H ₄	28.1	0.45	---	-0.45	-0.45	-0.45	-0.45
C ₂ H ₃ Cl	62.5	0.45	1.00	1.00	1.00	1.00	1.00
O ₂	32.0	0.04	---	---	---	-0.26	-0.13
product value			\$0.45	\$0.58	\$0.58	\$0.45	\$0.45
reactant cost			-\$0.71	-\$0.24	-\$0.24	-\$0.34	-\$0.22
excess value			-\$0.26	\$0.34	\$0.34	\$0.11	\$0.23

I/O diagram
for process
5 is shown
on slide 24

The bottom line represents \$/kg. If we know the kg/year, then we know the annual cash flow.

Problem 4.13

(a) Analyze the basic economics and show an I/O diagram for producing hydrogen from water, coal, and natural gas.

(b) What production mode (batch or continuous) should be used to obtain production rates of 2×10^7 and 1×10^8 kg/y?

Electricity:	\$0.05/kW·h
H ₂ :	\$4.67/kg (current market price of hydrogen)
O ₂ :	\$0.04/kg (Kirk-Othmer)
Coal:	\$0.055/kg
Steam:	\$0.008/kg
NG:	\$0.13/kg

References are Kirk-Othmer and Ullman's

basis: 1kg of H₂

Use same approach as Example 4-13

Continuous versus Batch

page 132-133

Batch if:

production rate < 50 m.t./y

heavy fouling

biological processes

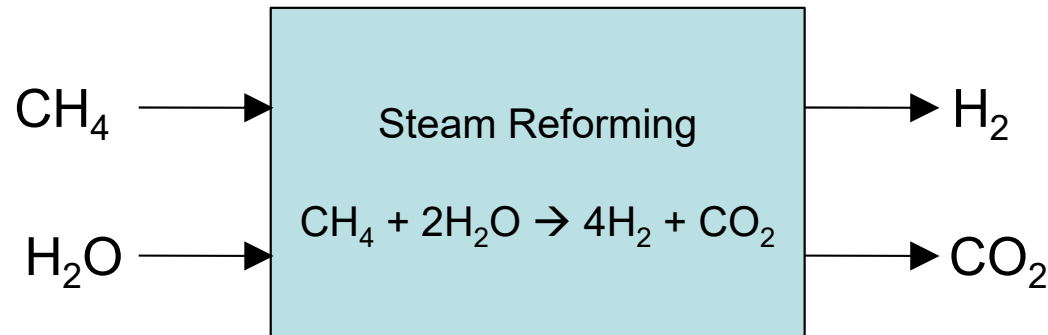
pharmaceutical processes

short product life spans, 1-2 y

product value \gg product cost

Problem 4.13

(a) Analyze the basic economics and show an I/O diagram for producing hydrogen from water, coal, and natural gas. (b) What production mode should be utilized to obtain production rates of 3×10^7 and 1×10^8 kg/yr?



basis: 1kg of H_2

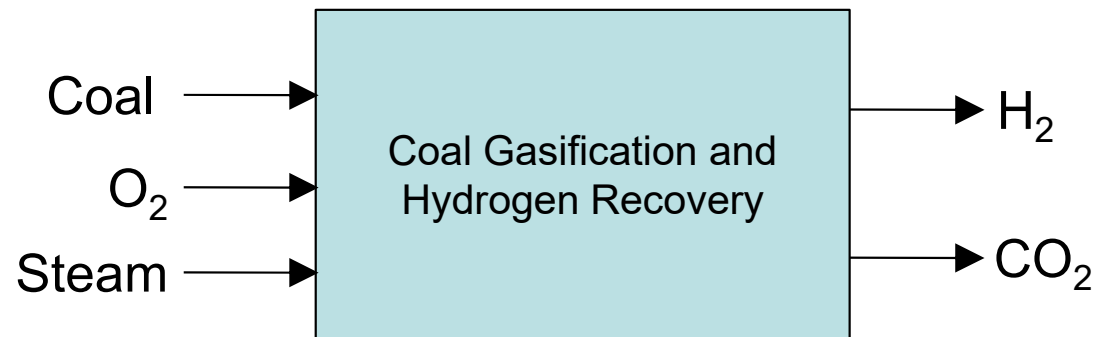
H_2 :	\$.67/kg (Kirk-Othmer)
O_2 :	\$.04/kg (Kirk-Othmer)
Steam:	\$.008/kg
NG:	\$.13/kg

Problem 4.13

Analyze the basic economics and show an I/O diagram for producing hydrogen from water, coal, and natural gas.

Need stoichiometry (reaction coefficients).

Also need an empirical formula for coal (coal is not "C").



basis: 1kg of H₂

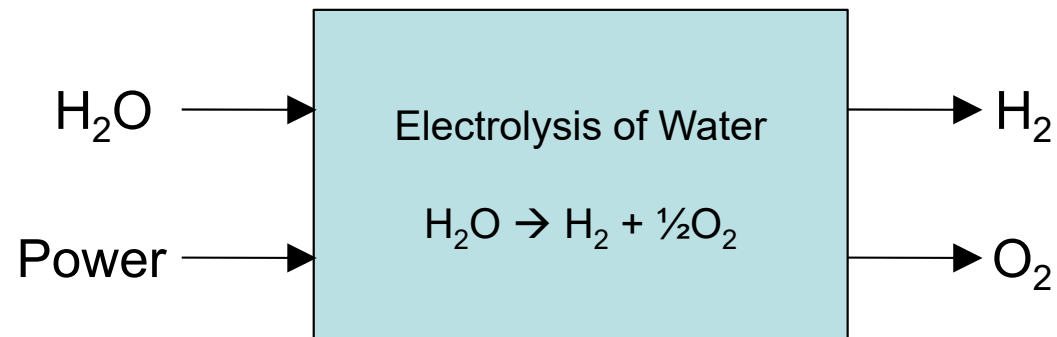
H ₂ :	\$.67/kg (Kirk-Othmer)
O ₂ :	\$.04/kg (Kirk-Othmer)
Coal:	\$.055/kg
Steam:	\$.008/kg

Problem 4.13

Analyze the basic economics and show an I/O diagram for producing hydrogen from water, coal, and natural gas.

Need a relationship between electrical power and stoichiometry

electrolysis is a cathode/anode process with 2 mol e⁻ flowing per mol H₂
think electrochemical (Daniel) cell from general chemistry with a voltage of ~1.23 V

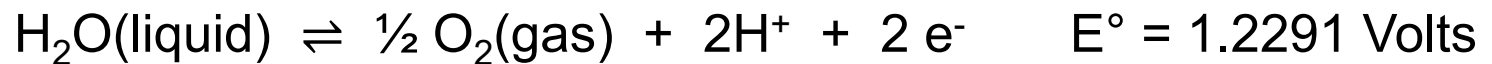


basis: 1kg of H₂

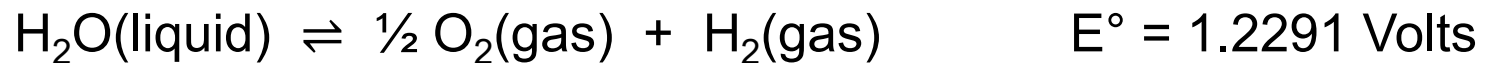
Electricity:	\$.05/kW·h
H ₂ :	\$.67/kg (Kirk-Othmer)
O ₂ :	\$.04/kg (Kirk-Othmer)

Balancing Electrochemical Reactions (General Chemistry)

Adding half-reactions:



Overall (water electrolysis):



In[1]:= (*Electric Power*)

$$\left(\frac{1 \text{ kmol_H2}}{2.0158 \text{ kg_H2}} \right) \left(\frac{2 \text{ kmol_e}}{1 \text{ kmol_H2}} \right) \left(\frac{1000 \text{ mol_e}}{1 \text{ kmol_e}} \right) \left(\frac{96485 \text{ C}}{1 \text{ mol_e}} \right) \left(\frac{1 \text{ Amp}}{1 \text{ C / s}} \right) * 1.2291 \text{ V} \left(\frac{1 \text{ W}}{1 \text{ V} * \text{Amp}} \right) \left(\frac{1 \text{ kW}}{1000 \text{ W}} \right) \left(\frac{1 \text{ h}}{3600 \text{ s}} \right)$$

Out[1]= $\frac{32.68339 \text{ h kW}}{\text{kg_H2}}$

Questions?