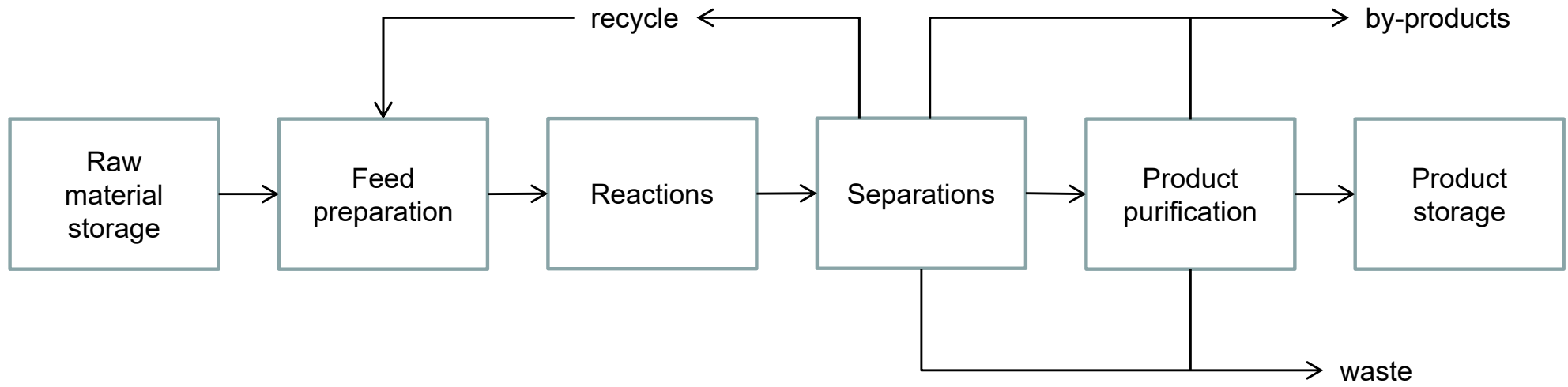


CH402 Chemical Engineering Process Design

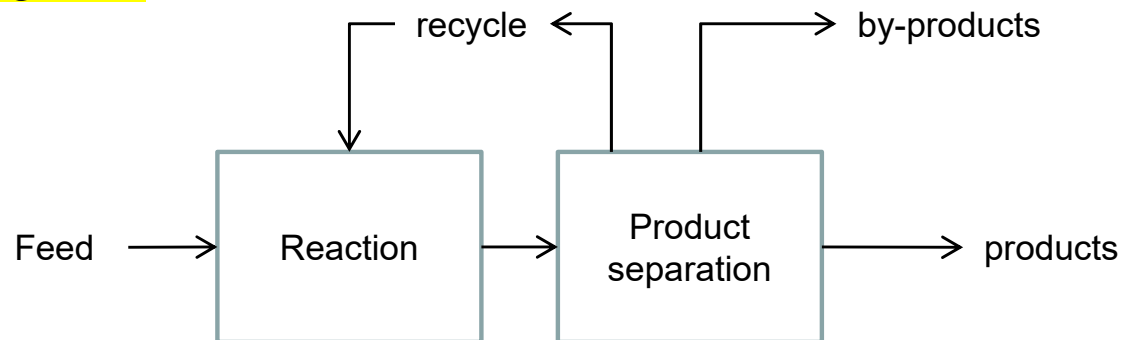
Class Notes L13

Flowsheet Synthesis

Block Diagram of (all) Chemical Processes



“Functions Diagram”



Q's may or may not be shown

Often simplified to this form.

Case Study - Vinyl Chloride Monomer (VCM) Production

Problem definition (market survey)

21,100,000 tons/y in 2000

3.7% growth from 2000-2009

40,000,000 tons/y in 2009

2.7% growth from 2009-2024

8,000,000 t/y in 2009

12 US plants

~10,000,000 t/y in 2020

Emissions are a problem

23 Feb 2023 East Palestine, OH

average US plant capacity is 667,000 t/y

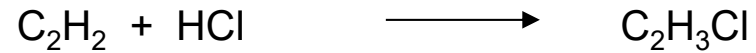
1,334 million lbs/y per plant
604.8 million kg/y per plant

Known Vinyl Chloride Routes

Next step is a literature search – 5 Routes Identified

Kirk-Othmer, Wikipedia

(also CH383)



Route 1

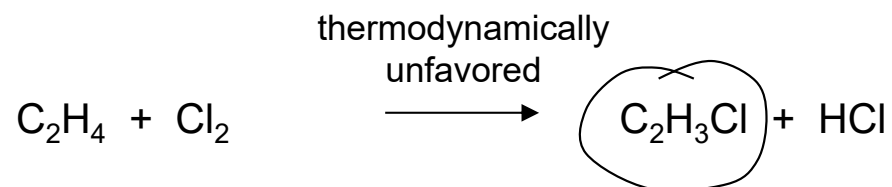
direct reaction of acetylene
(acetylene hydrochlorination)

Known Vinyl Chloride Routes

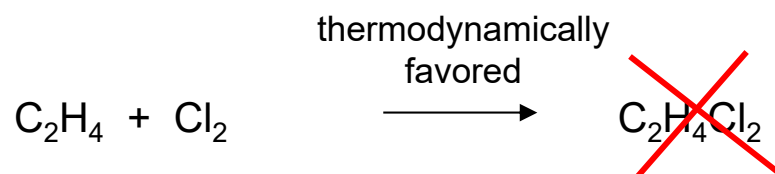
Kirk-Othmer, Wikipedia

Literature Search

(also CH383)



Route 2
direct chlorination of
ethylene (liquid phase)



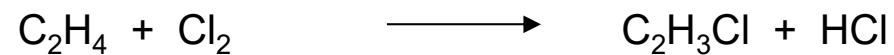
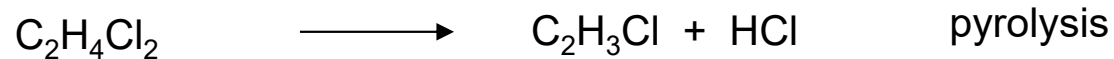
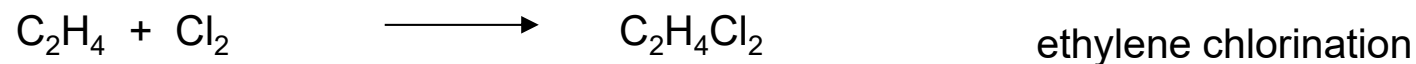
Not the product we want

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

Literature Search

CH383

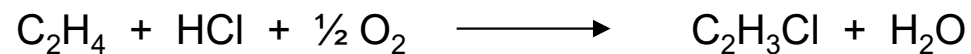
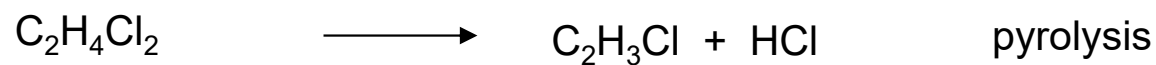


Route 3
direct chlorination + pyrolysis

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

Literature Search



Route 4
oxychlorination + pyrolysis

Known Vinyl Chloride Routes

Kirk-Othmer, Wikipedia

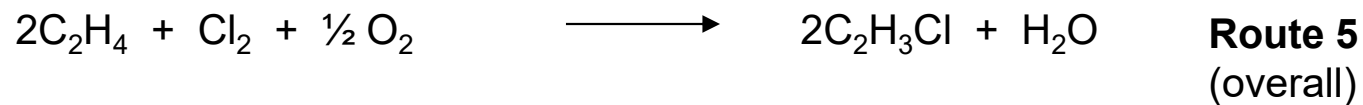
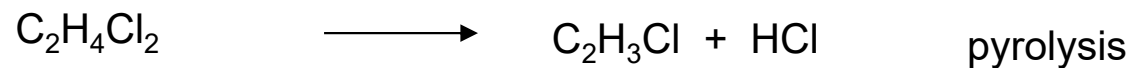
Literature Search



+



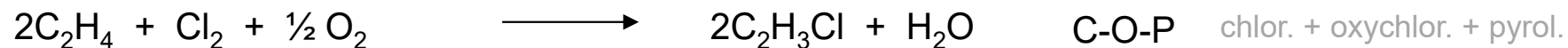
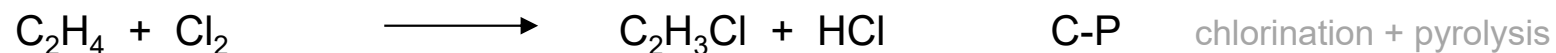
+



Known Vinyl Chloride Routes

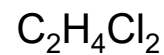
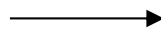
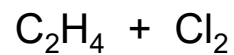
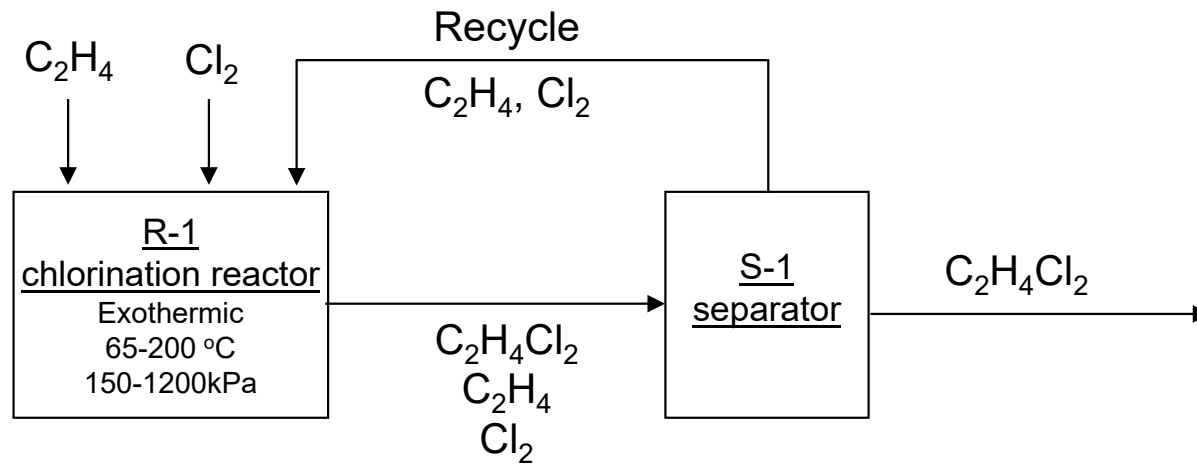
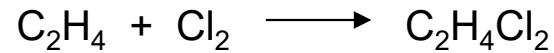
5 processes identified in literature survey

Summary



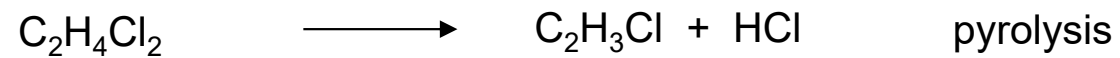
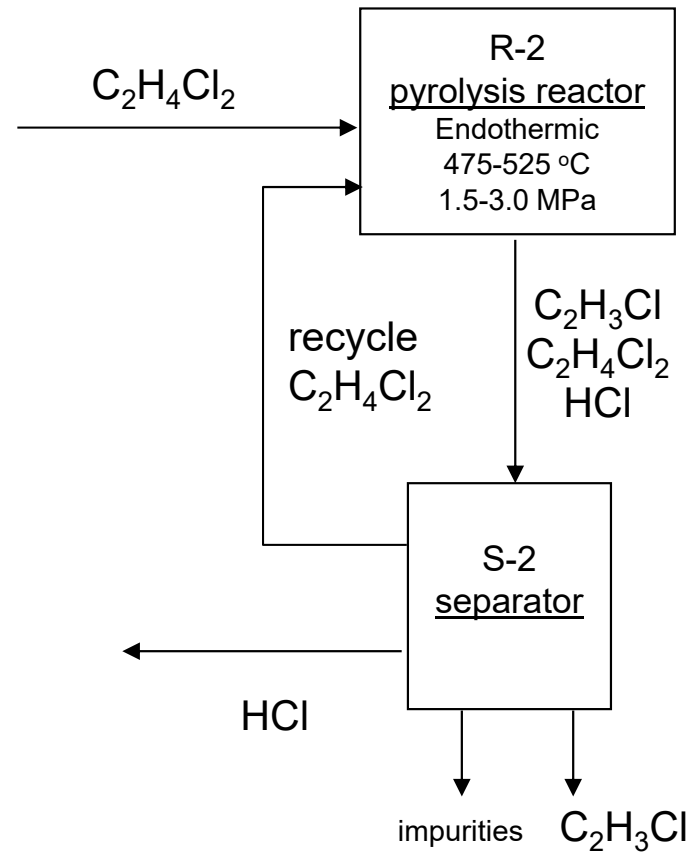
Functions Diagram – C – Direct Chlorination

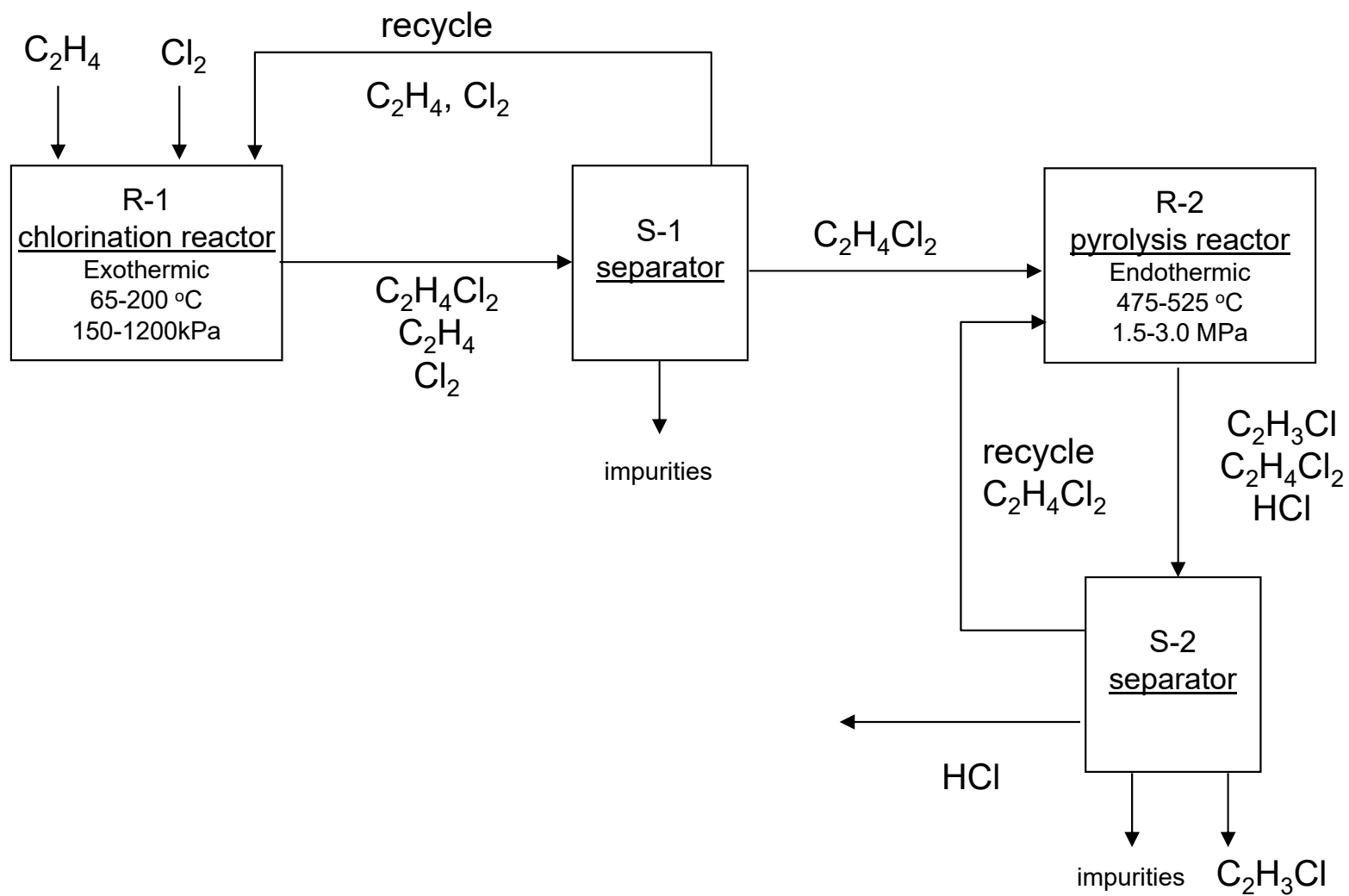
The utility of the functions diagram is that it can be used to build much larger processes.



ethylene chlorination

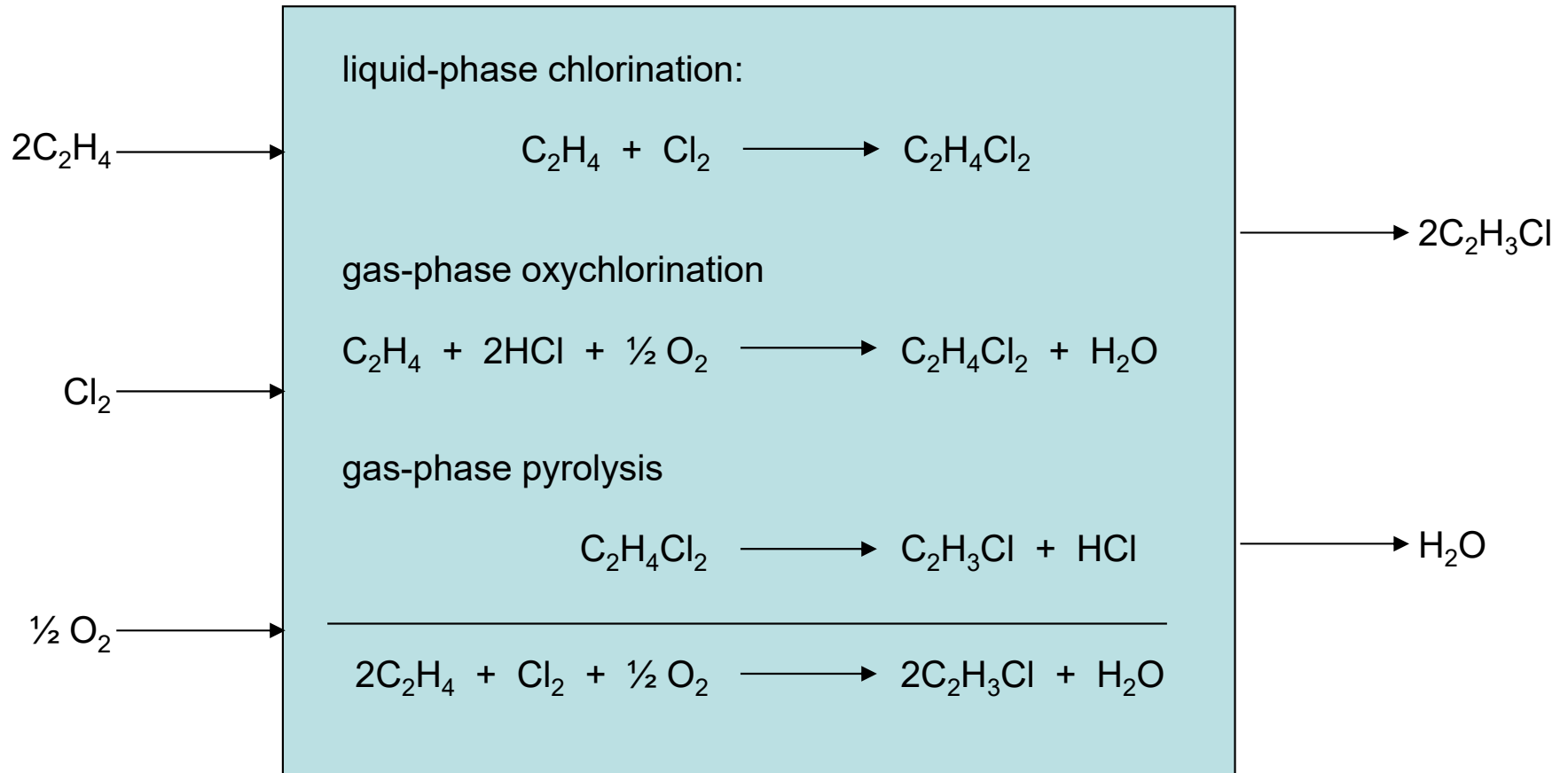
Functions Diagram – Pyrolysis





Input/Output Structure - Route 5 - COP

I/O box is frequently left blank



The I/O analysis allows us to make an assessment of 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.

2 pts bonus – complete table in Excel – submit with PS6 - (pdf of table only)

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

Electricity:	\$.05/kW·h
H ₂ :	\$.67/kg (Kirk-Othmer)
O ₂ :	\$.04/kg (Kirk-Othmer)
Coal:	\$.055/kg
Steam:	\$.008/kg
NG:	\$.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

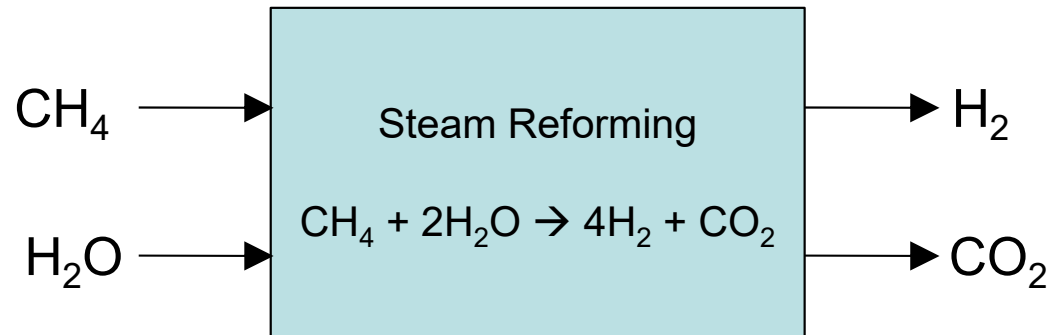
pharmaceutical processes

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

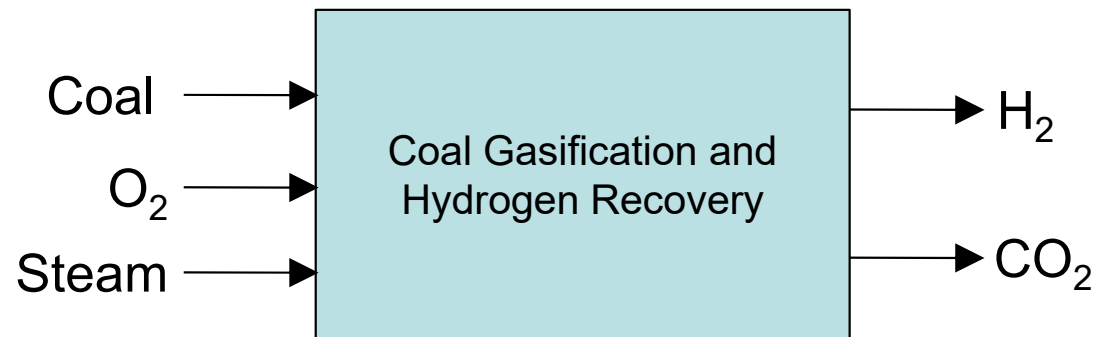
H_2 :	\$.67/kg (Kirk-Othmer)
O_2 :	\$.04/kg (Kirk-Othmer)
Steam:	\$.008/kg
NG:	\$.13/kg

Problem 4.13

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

hint 1: need stoichiometry (reaction coefficients).

hint 2: need an empirical formula for coal (coal is not "C").



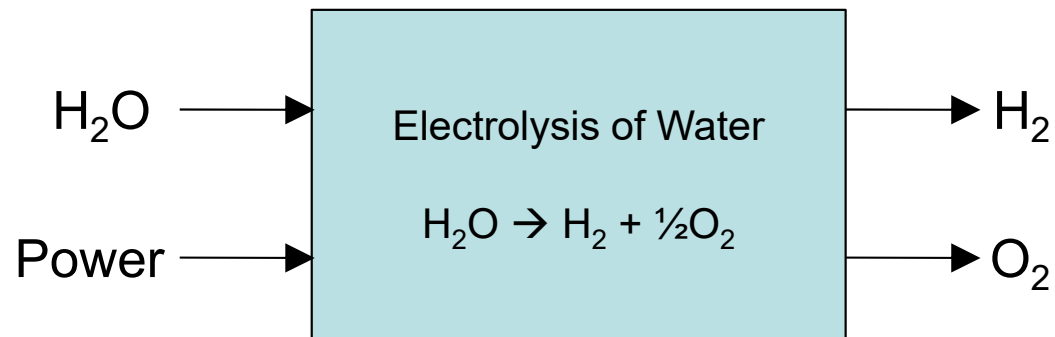
basis: 1kg of H₂

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.

hint: need a relationship between electrical power and stoichiometry



basis: 1kg of H_2

electrolysis is a cathode/anode process with 2 mol e^- flowing per mol H_2
think electrochemical (Daniel) cell from general chemistry with a voltage of $\sim 1.1 \text{ V}$

Electricity:	\$.05/kW·h
H_2 :	\$.67/kg (Kirk-Othmer)
O_2 :	\$.04/kg (Kirk-Othmer)

Questions?