# EngrD 2190 – Lecture 8

Concept: Process Analysis – Mass Balances with Chemical Reactions

Context: Options for Unreacted Reactants:

Discard?

Separate & Recyle?

Recycle with Purge?

Defining Question: What are the two options for writing a mass balance on a system with chemical reactions?

Read Chapter 3 pp. 106-110 (mass balances with chemical reactions)

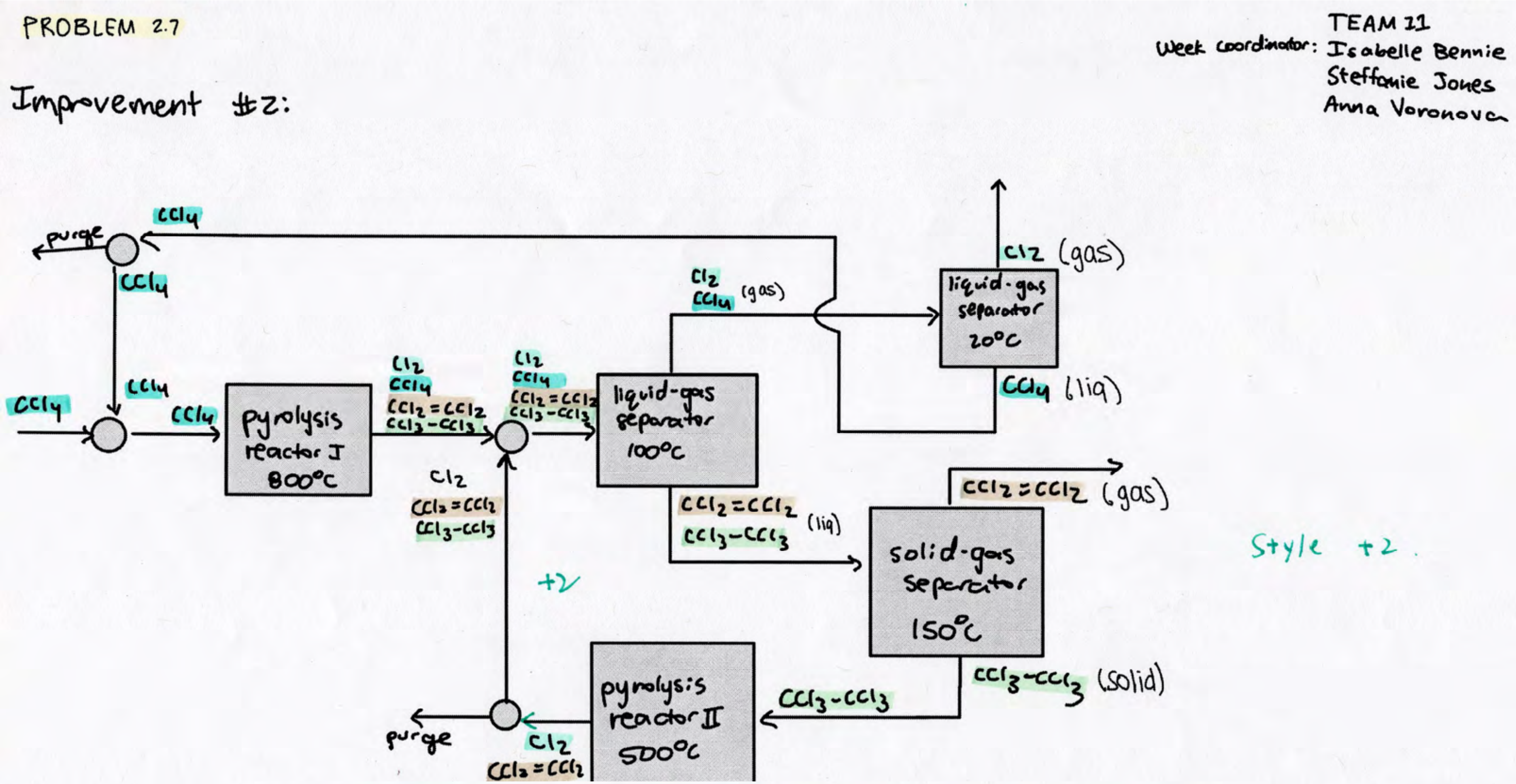
# EngrD 2190 – Lecture 8

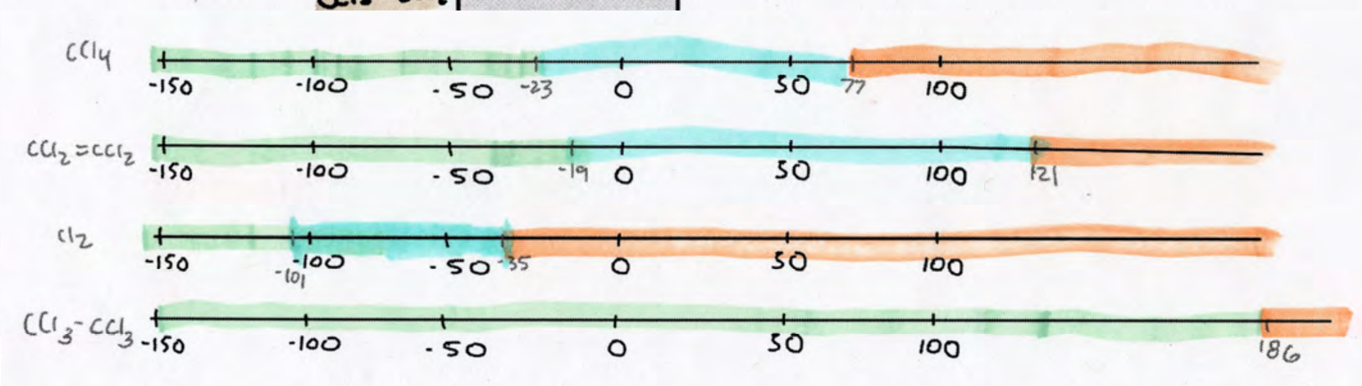
- Homework 2 due today at noon.

Write team code and names of all *contributing* team members on all solutions. Indicate this week's Team Coordinator.

Submit *after* lecture or deliver to the EngrD 2190 mailbox in a cabinet in the hallway outside 116 Olin Hall (ChemE Business Office). **Not to my mailbox.**

# Homework 1 Excellence – exercise 2.7 – Team 11



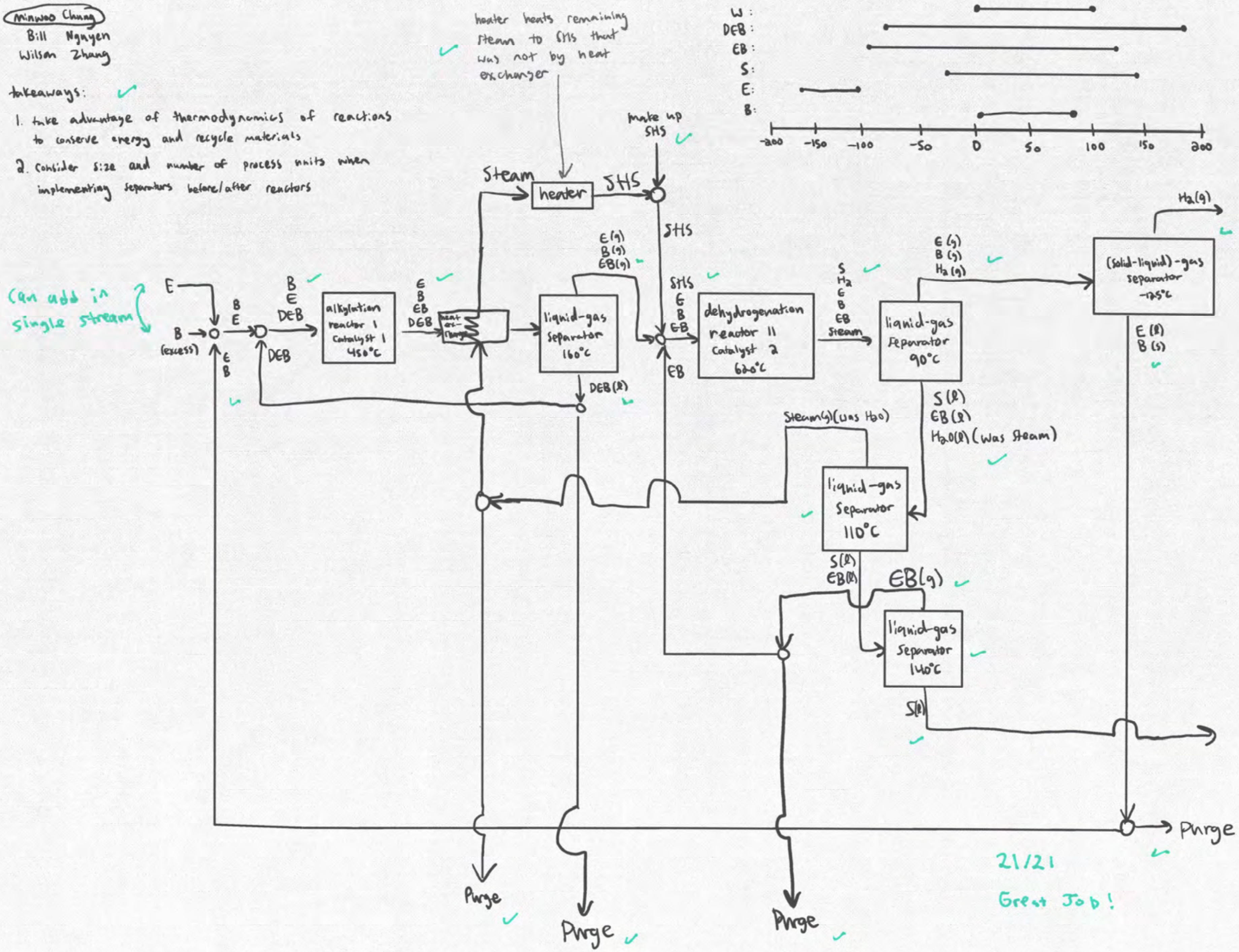
# Homework 1 Excellence – exercise 2.24 – Team 6

2.24

Minwoo Chung
Bill Nguyen
Wilson Zhang

takeaways: ✓

1. take advantage of thermodynamics of reactions to conserve energy and recycle materials
2. consider size and number of process units when implementing separators before/after reactors

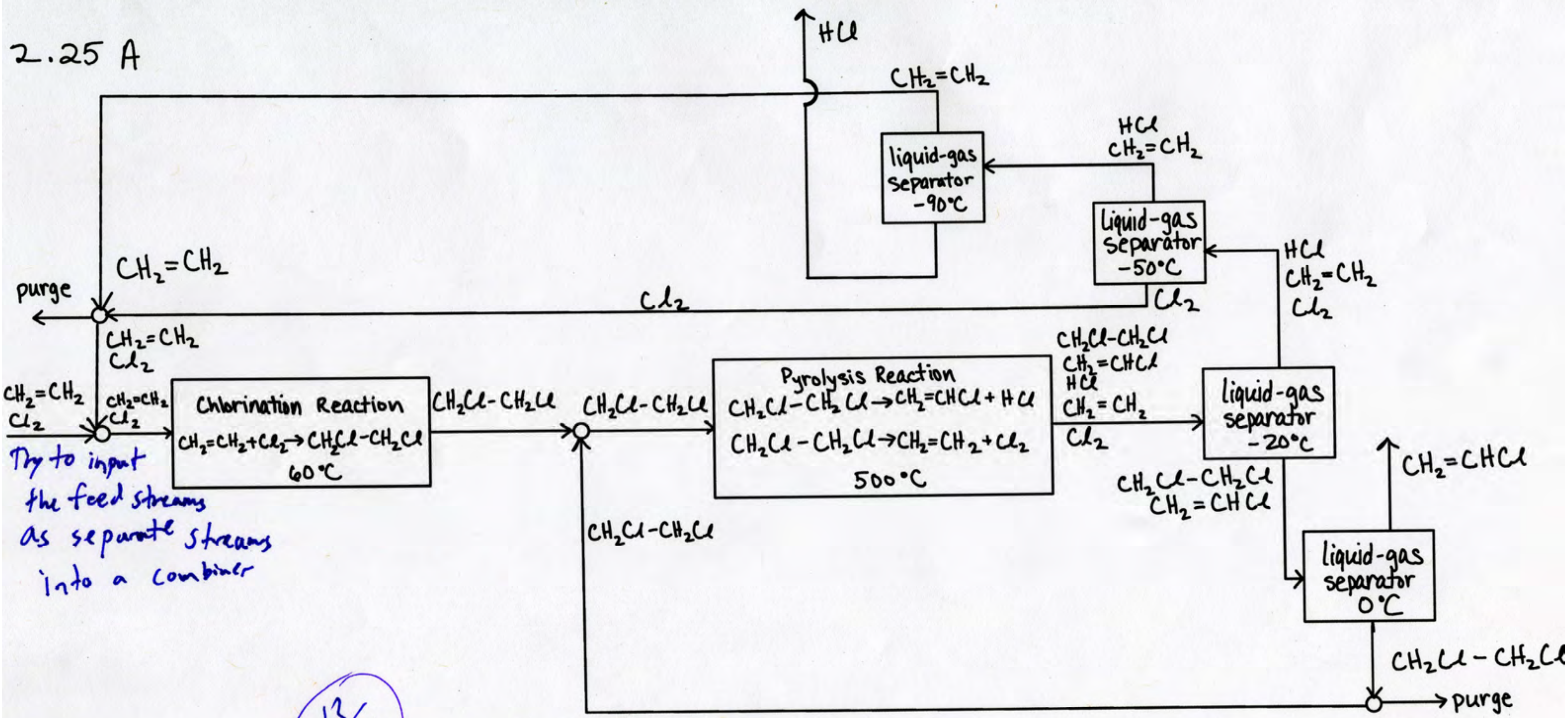


# Homework 1 Excellence – exercise 2.25(A) – Team 18

Amber Belk (Coordinator), Dolly Hritz, Parth Vaidyanath

Team 18

2.25 A




13/13 Good job!

Key Takeaways:

- You can have multiple reactions in a reactor.
- If there is another reaction that uses some of the product with a low conversion rate (i.e., 35%), it is not worth the extra process unit. The extra reactions are cyclical so they are useless to use
- When separating many compounds, it is better to separate the compounds approximately in half so that further separators are smaller.

# EngrD 2190 – Lecture 8

- Homework 3 due Friday 9/19:

  Formal mass balances:

  **exercises 3.12 and 3.28**

  *Every equation must have an explicit source.*

  see posted solutions for exercises 3.4, 3.10, and 3.24 (calculation session 3) and exercise 3.44 (today's lecture).

  *Append a list of 'take-aways' to each exercise.*

  Process Design with qualitative, informal mass balances:

  **exercises 3.115 and 3.125**

  see posted solutions for exercises 2.36 and 3.126 (lecture 6), exercises 2.32 (calculation session 2), and 2.35 (calculation session 3).

  *Append a list of 'take-aways' to each exercise.*

***Start each solution on a separate page.***

# Requirements for Formal Mass Balances

- Define nomenclature.
- Show system borders and state assumptions.
- State source of equations. ***Every** equation must have an explicit source.*

  examples: "apply conservation of mass" or "stream compositions" or "process specification for washer"
- Describe derivation. "Substitute eqns (1) and (2) into eqn (3)."
- Box your answers. Numbers must have proper significant figures and include units (e.g., kg/min).

Flow sheets for mass balance exercises are posted on-line.

Select the "Textbook" item at the EngrD 2190 homepage.

# Exercise 2.35

**2.35** Design a process to produce $P$ from $A$. (Not the same $A$ and $P$ as in any other exercise.)

$$A \leftrightarrow P$$

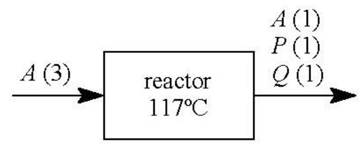
The reaction is reversible; $P$ can be converted to $A$. $A$ also reacts reversibly to form $Q$.

$$A \leftrightarrow Q$$

The reactions of $A$ to form $P$ and $Q$ go to equilibrium, which is an equimolar mixture of $A$, $P$, and $Q$.

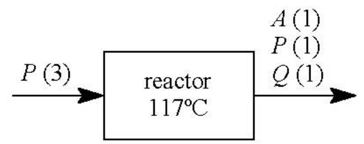
Deductive

The example below shows the reactor effluent when pure $A$ enters the reactor. The numbers in parentheses are flow rates, in mol/min.




Inductive

*Any* composition of $A$, $P$, and $Q$ entering the reactor will leave as an equimolar mixture of $A$, $P$, and $Q$. For example,

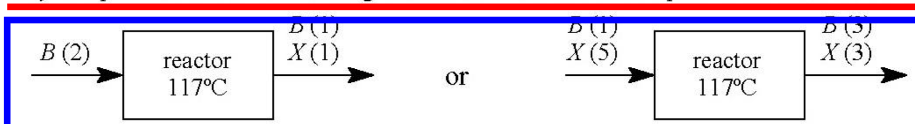



$A$ is available only as a mixture of 90% $A$ and 10% $B$. (All compositions in this exercise are in mol%.) The reactor that converts $A$ to $P$ (and $Q$) also converts $B$ to $X$.

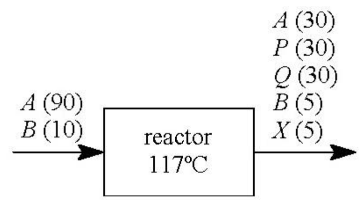
$$B \leftrightarrow X$$

*Any* composition of $B$ and $X$ entering the reactor will leave as an equimolar mixture of $B$ and $X$.

Deductive




In summary, 100 mol of feed entering the reactor will produce the following output.




Inductive

Design Goals (in decreasing importance)

- Maximize the total value of the product(s).
- Minimize the *number* of units.
- Minimize the *size* of each unit.

Design Rules.

- Start with 100. mol/min of a 90:10 $A$:$B$ mixture.
- List the substances and *approximate* flow rates in every stream. One significant figure is sufficient.

# Exercise 2.35 with deductive only

**2.35** Design a process to produce $P$ from $A$. (Not the same $A$ and $P$ as in any other exercise.)

$$A \leftrightarrow P$$

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# *News Item*

*Walk this number of steps each day to cut your risk of dementia*

By Sandee LaMotte, CNN, September 6, 2022

… People between the ages of 40 and 79 who took 9,826 steps per day were 50% less likely to develop dementia within seven years, the study found. Furthermore, people who walked with "purpose" – at a pace over 40 steps a minute – were able to cut their risk of dementia by 57% with just 6,336 steps a day.

The standard step length is 2.5 ft. The original study likely specified 'walking with purpose' a distance of 3 miles.

$$3 \text{ miles} \times (5280 \text{ ft/mile}) \div (2.5 \text{ ft/step}) = 6336 \text{ steps}$$

Try walking 'without purpose' – fewer than 40 steps per minute.

# Options for Unreacted Reactants

valuable Product

worthless By-product

$$A \rightarrow P + B$$

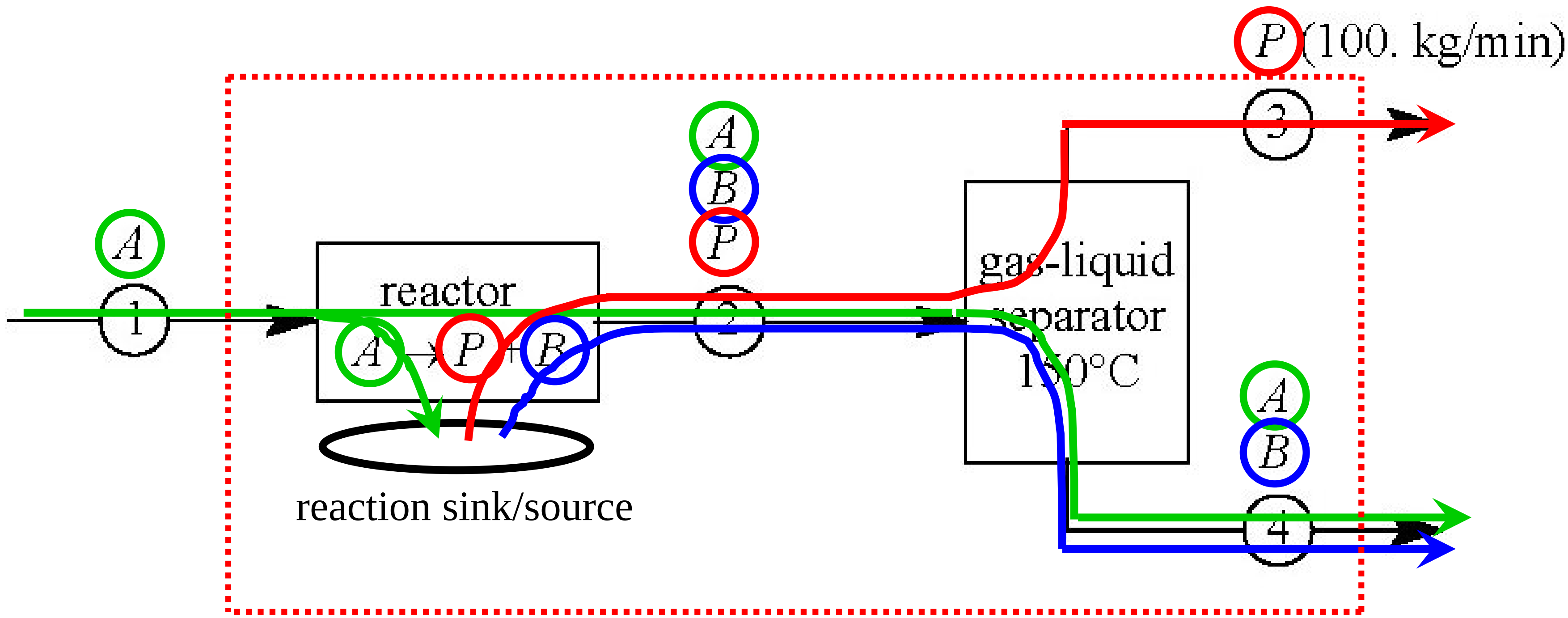
| | b.p. |
|---|---|
| A | 180°C |
| B | 181°C |
| P | 120°C |

small $\Delta T$; difficult separation

large $\Delta T$; easy separation

Scheme I. Avoid the expensive separator. Discard unreacted $A$ with by-product $B$.

Model 1: one border should cross stream 3 - flow rate and composition given.




Model 1: (3 streams) × (3 parameters/stream) = 9 parameters

Calculate the flow rate and composition of stream 4. Calculate the flow rate of stream 1.

Scheme I is a simple process. It is tempting to calculate informally.

Instead, we will use this as an example of formal mathematically modeling.

# A Formal Mathematical Model

Translate the process flowsheet to equations.

Identify a Physical Law or a Process Specification.

Translate to an equation.

Solve the equations.

Describe your method.

"Substitute equations (1) and (2) into equation (3)."

Show a logical mathematical progression.

$$2F_{T,1} + 32 = F_{T,2}$$

$$2F_{T,1} = F_{T,2} - 32$$

$$F_{T,1} = \frac{F_{T,2} - 32}{2}$$

*Every* equation must have an explicit source.

# Model 1 of Scheme I – Mathematical Model

Choose a set of parameters. Choose 3 parameters from 4: total, *A*, *B*, and *P*.

1. Total and 2 components; probably total, *A*, and *P*.
2. 3 components; *A*, *B*, and *P*. arbitrarily choose this.

Translate the process flowsheet to equations.

Apply the Conservation of Mass to *P*. Write a mass balance on *P*.

rate of *P* in = rate of *P* out

$$F_{P,1} = F_{P,3} + F_{P,4}$$

$$0 \cancel{=} 100 + 0$$

Implies system with red borders and process at steady state.

If you choose to omit this equation, you must *explicitly* describe system borders and state assumptions.

What is wrong? Although mass is conserved, *P* is not.

Closed system: $\boxed{A}$ initially $\boxed{A + B + P}$ later

# Model 1 of Scheme I – Mathematical Model, cont'd

Apply the Conservation of Mass to $P$. Write a mass balance on $P$.

rate of $P$ in + rate $P$ is created = rate of $P$ out + rate $P$ is consumed

Second option: explicitly list the source from which $P$ is created and the sink to which $P$ is consumed.

For $A \rightarrow P + B$,

rate of $P$ in + rate of $A$ in + rate of $B$ in = rate of $P$ out + rate of $A$ out + rate of $B$ out

Arbitrarily choose the second option.

$$F_{P,1} + F_{A,1} + F_{B,1} = F_{P,3} + F_{P,4} + F_{A,3} + F_{A,4} + F_{B,3} + F_{B,4} \qquad (1)$$

Process Specifications: stream 1: $F_{P,1} = F_{B,1} = 0$ (2), (3)

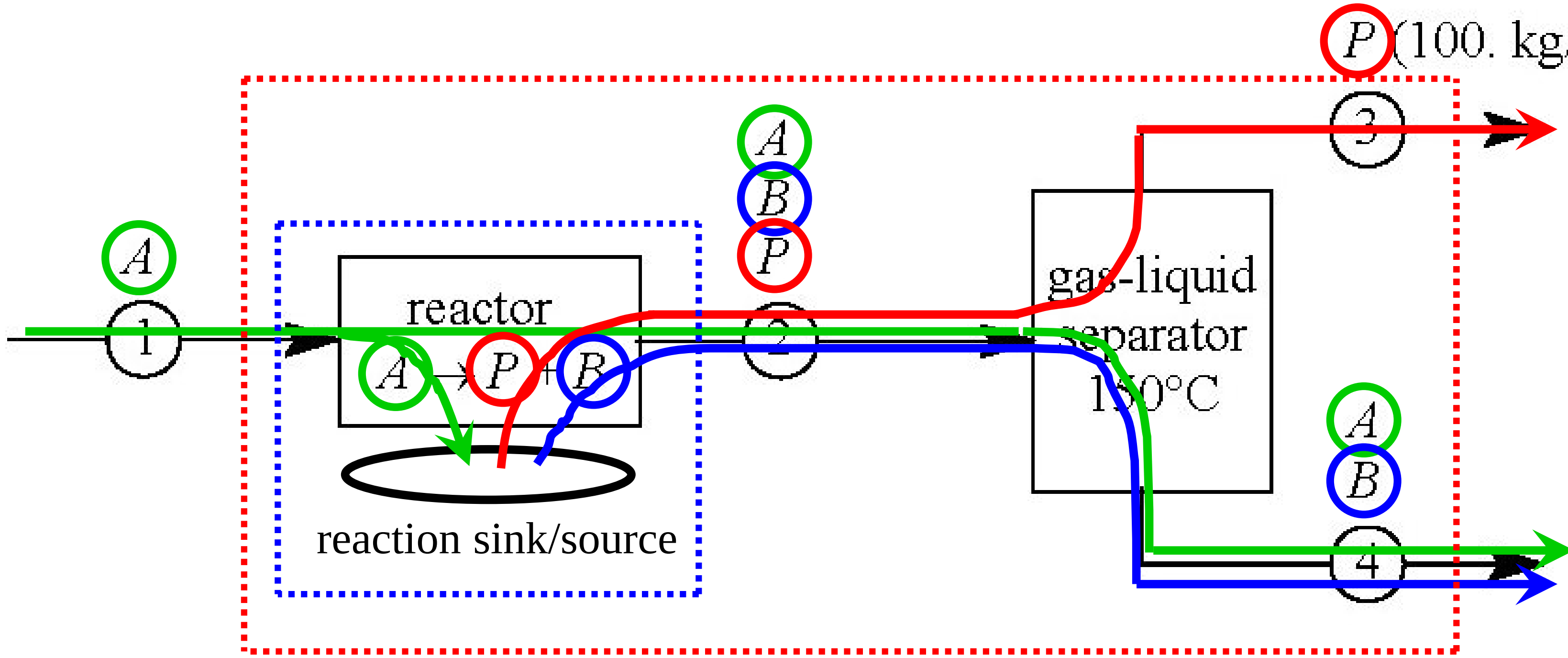
stream 3: $F_{A,3} = F_{B,3} = 0$, $F_{P,3} = 100.$ (4), (5), (6)

stream 4: $F_{P,4} = 0$ (7)

9 parameters, 7 equations $\Rightarrow$ need 2 more equations. *Consider the reactor.*

Scheme I. Avoid the expensive separator. Discard unreacted $A$ with by-product $B$.

Model 1: one border should cross stream 3 - flow rate and composition given.




Model 1: (3 streams) × (3 parameters/stream) = 9 parameters

Calculate the flow rate and composition of stream 4. Calculate the flow rate of stream 1.

Model 2: (2 streams) × (3 parameters/stream) = 6 parameters

# Model 2 of Scheme I – Mathematical Model

Reaction Specification: 60% of *A* reacts (40% does not) deductive

inductive: assume 100 kg of *A* enters reactor $\Rightarrow$ 40 kg of *A* leaves the reactor.

$\Rightarrow$ 60 kg of *P* + *B* leaves the reactor.

$$0.40F_{A,1} = F_{A,2} \quad (2.1)$$

$$0.60F_{A,1} = F_{P,2} + F_{B,2} \quad (2.2)$$

What are the relative masses of *P* and *B* created?

mol wt $P = 2 \times$ (mol wt $B$) deductive

If the mol wt of *P* is 100 amu, the mol wt of *B* is 50 amu inductive

If the mass of *P* + *B* created is 150 kg, *P* is 100 kg and *B* is 50 kg.

If the mass of *P* + *B* created is 60 kg, *P* is 40 kg and *B* is 20 kg.

$$F_{P,2} = 2F_{B,2} \quad (2.3)$$

# Model 2 of Scheme I – Mathematical Model, cont’d

$$F_{P,2} = 2F_{B,2} \qquad (2.3)$$

Equation (2.3) can also be obtained with a reactor mass balance.

$$\text{rate of } P \text{ in} + \text{rate } P \text{ is created} = \text{rate of } P \text{ out} + \text{rate } P \text{ is consumed}$$

$$\cancelto{0}{F_{P,1}} + (2/3)(0.60F_{A,1}) = F_{P,2} + 0$$

$$0.40F_{A,1} = F_{P,2}$$

$$\text{rate of } B \text{ in} + \text{rate } B \text{ is created} = \text{rate of } B \text{ out} + \text{rate } B \text{ is consumed}$$

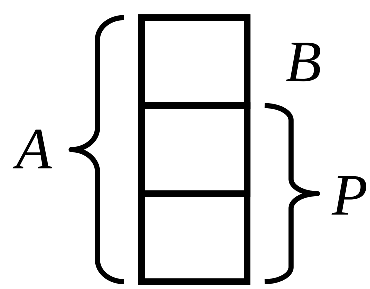
$$\cancelto{0}{F_{B,1}} + (1/3)(0.60F_{A,1}) = F_{B,2} + 0$$

$$0.20F_{A,1} = F_{B,2}$$

$$F_{P,2} = 2F_{B,2} \qquad (2.3) \qquad \text{informal}$$

Equation (2.3) can also be obtained visually.

$$A \rightarrow P + B \;\text{ and }\; \text{mol wt } P = 2(\text{mol wt } B)$$



# Model 3 of Scheme I

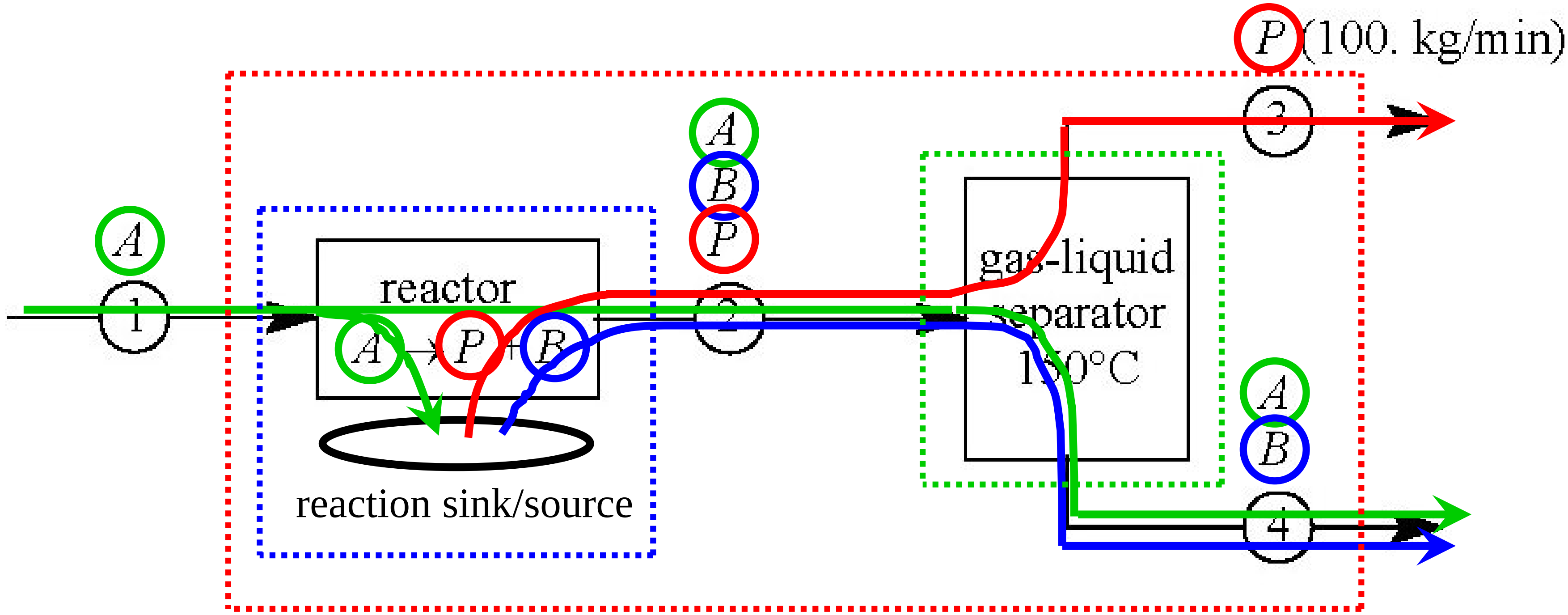
How to relate stream 2 (internal) to external streams?

We need a system with a border that crosses stream 2 and a border that crosses a known external stream.

Draw system borders around the separator.

Scheme I.   Avoid the expensive separator.  Discard unreacted $A$ with by-product $B$.

Model 1:  one border should cross stream 3 - flow rate and composition given.




Model 1:  (3 streams) × (3 parameters/stream) = 9 parameters

Calculate the flow rate and composition of stream 4.  Calculate the flow rate of stream 1.

Model 2:  (2 streams) × (3 parameters/stream) = 6 parameters

Model 3:  (3 streams) × (3 parameters/stream) = 9 parameters

# Model 3 of Scheme I – Mathematical Model

Write a mass balance on the separator (note: no chemical reactions).

rate of *A* in = rate of *A* out

$$F_{A,2} = \cancelto{0}{F_{A,3}} + F_{A,4} \quad \text{(informal)}$$

$$F_{A,2} = F_{A,4} \quad (3.1)$$

Substitute equation (3.1) into equation (2.1).

$$0.4F_{A,1} = F_{A,2} \quad (2.1)$$

$$0.4F_{A,1} = F_{A,4} \quad (8)$$

Substitute equation (2.3) ($F_{P,2} = 2F_{B,2}$) into equation (2.2).

$$0.60F_{A,1} = F_{P,2} + F_{B,2} \quad (2.2)$$

$$0.60F_{A,1} = 2F_{B,2} + F_{B,2}$$

$$0.60F_{A,1} = 3F_{B,2} \quad (2.4)$$

# Model 3 of Scheme I – Mathematical Model, cont'd

Write a mass balance on the separator (note: no chemical reactions).

rate of *B* in = rate of *B* out

$$F_{B,2} = \cancelto{0}{F_{B,3}} + F_{B,4} \quad \text{(informal)}$$

$$F_{B,2} = F_{B,4} \quad (3.2)$$

Substitute equation (3.2) into equation (2.4).

$$0.60F_{A,1} = 3F_{B,2} \quad (2.4)$$

$$0.60F_{A,1} = 3F_{B,4}$$

$$0.20F_{A,1} = F_{B,4} \quad (9)$$

We now have 9 equations for System 1 (borders around entire process).

# Model 1 of Scheme I – Mathematical Model

$$F_{P,1} + F_{A,1} + F_{B,1} = F_{P,3} + F_{P,4} + F_{A,3} + F_{A,4} + F_{B,3} + F_{B,4} \quad (1)$$

stream 1: $F_{P,1} = 0$ (2)

$F_{B,1} = 0$ (3)

stream 3: $F_{A,3} = 0$ (4)

$F_{B,3} = 0$ (5)

$F_{P,3} = 100.$ (6)

stream 4: $F_{P,4} = 0$ (7)

$0.4F_{A,1} = F_{A,4}$ (8)

$0.2F_{A,1} = F_{B,4}$ (9)

Substitute equations (2)-(7) into equation (1).

$$0 + F_{A,1} + 0 = 100 + 0 + 0 + F_{A,4} + 0 + F_{B,4}$$

$$F_{A,1} = 100 + F_{A,4} + F_{B,4} \quad (10)$$

Use equations (8) and (9) to substitute for $F_{A,4}$ and $F_{B,4}$ in equation (10).

$$F_{A,1} = 100 + 0.4F_{A,1} + 0.2F_{A,1}$$

$$(1 - 0.6)F_{A,1} = 100$$

$$F_{A,1} = 250 \text{ kg/min}$$

# Model 1 of Scheme I – Mathematical Model, cont'd

From the previous slide, $F_{A,1} = 250$ kg/min

Use equation (8) to calculate $F_{A,4}$.

$$F_{A,4} = 0.4F_{A,1} \quad (8)$$

$$F_{A,4} = 0.4(250) = 100 \text{ kg/min}$$

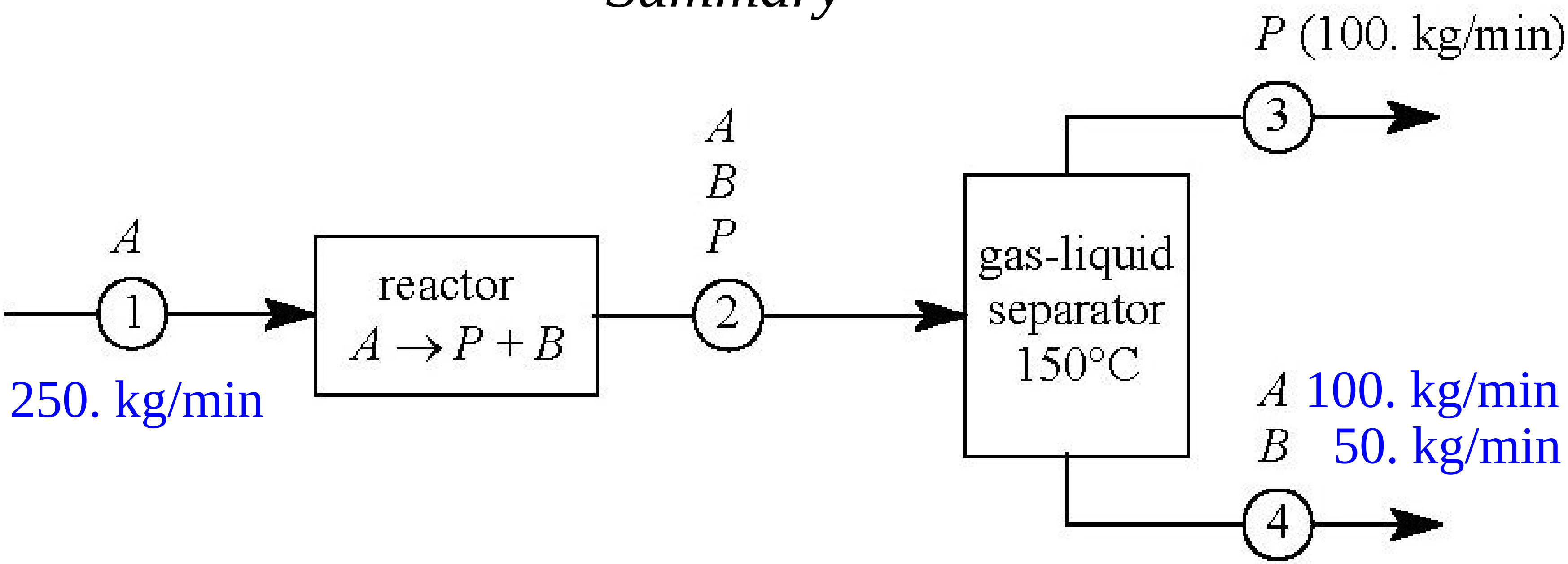
Use equation (9) to calculate $F_{B,4}$.

$$F_{B,4} = 0.20F_{A,1} \quad (9)$$

$$F_{B,4} = 0.20(250) = 50 \text{ kg/min}$$

Scheme I. Avoid the expensive separator. Discard unreacted *A* with by-product *B*.

*Summary*




Check Overall mass balance okay? In: 250 kg/min

Out: 100 + 100 + 50 = 250 kg/min ✓

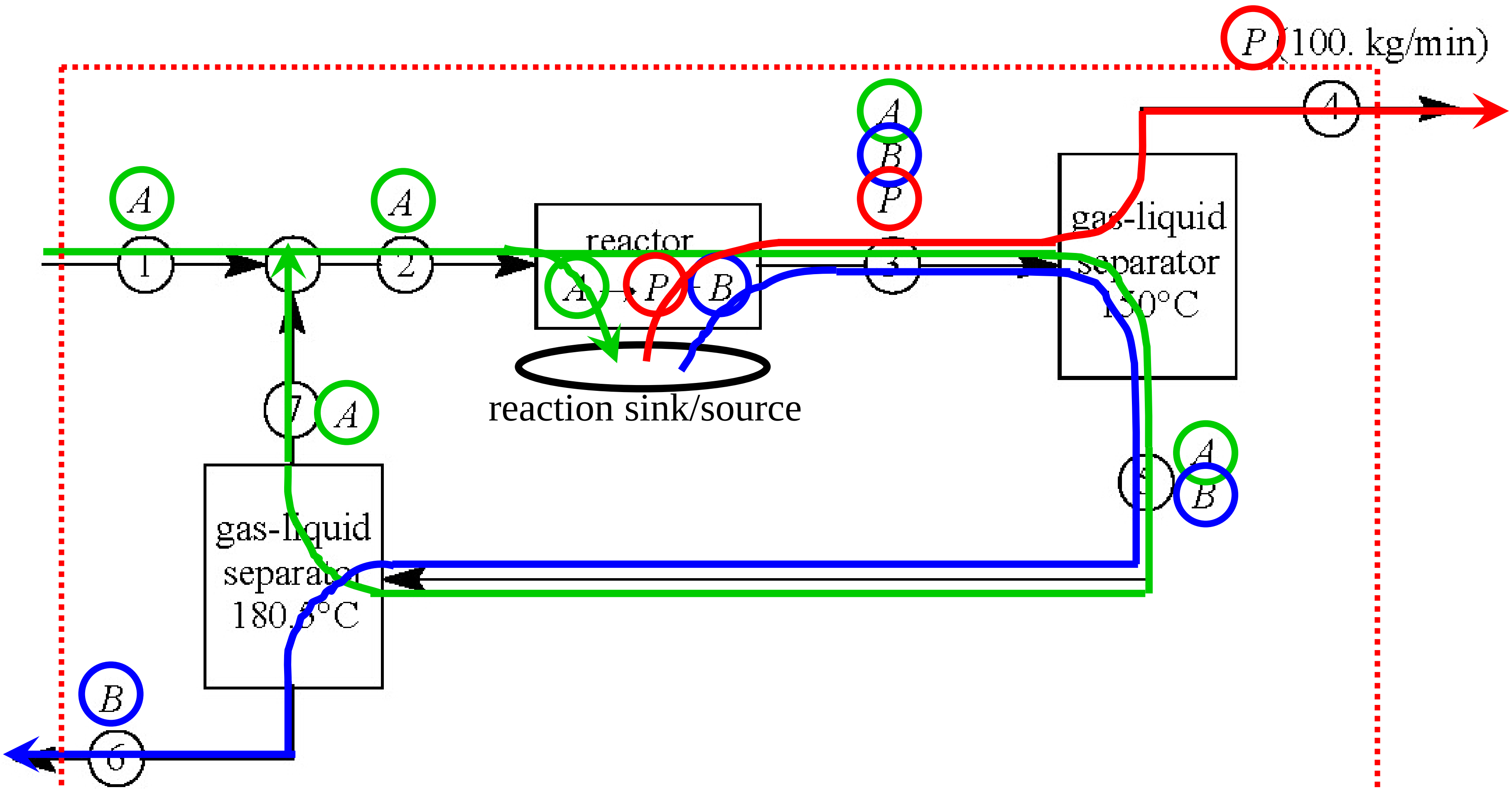
Mass ratio of *P* to *B* equals 2:1? *P* out = 100 kg/min

*B* out = 50 kg/min ✓

Scheme I is part (A) of exercise 3.44.

*Solution is posted.*

Scheme II. Separate unreacted *A* from by-product *B* and recycle *A*.




Model 1: (3 streams) × (3 parameters/stream) = 9 parameters

Calculate the flow rates of streams 1 and 6, in kg/min. Calculate the flow rate and composition of stream 3.

# Model 1 of Scheme II – Mathematical Model

Write a mass balance:

rate of *P* in + rate of *A* in + rate of *B* in = rate of *P* out + rate of *A* out + rate of *B* out

$$F_{P,1} + F_{A,1} + F_{B,1} = F_{P,4} + F_{P,6} + F_{A,4} + F_{A,6} + F_{B,4} + F_{B,6} \qquad (1)$$

Process Specifications: stream 1: $F_{B,1} = F_{P,1} = 0$ (2), (3)

stream 4: $F_{A,4} = F_{B,4} = 0,\ F_{P,4} = 100.$ (4), (5), (6)

stream 6: $F_{A,6} = F_{P,6} = 0$ (7), (8)

We need a 9th equation. Because only *A* enters the reactor, a mass balance on the reactor yields the analogous result as Scheme I:

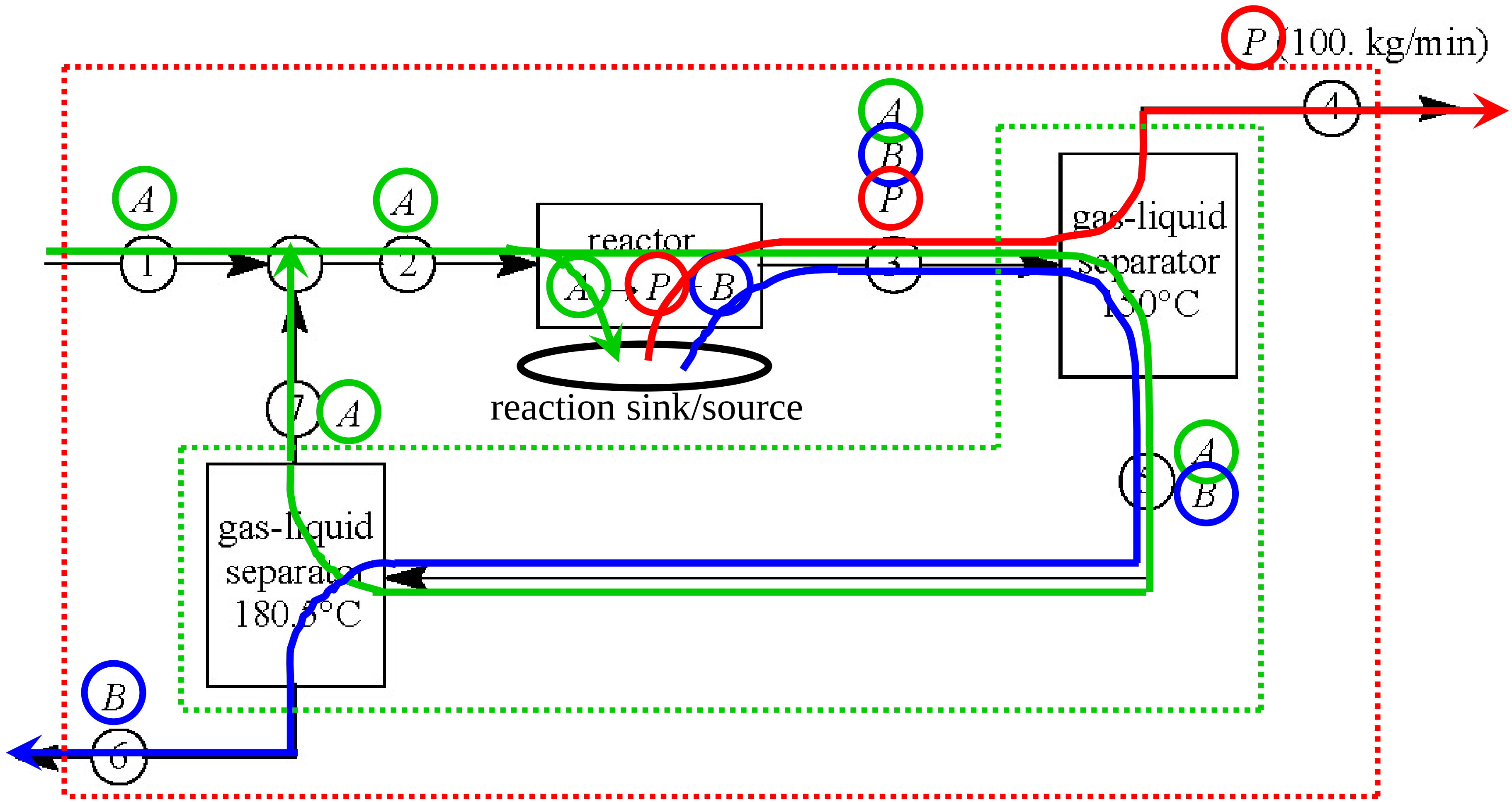
$$0.6F_{A,2} = F_{B,3} + F_{P,3} \qquad (2.1)$$

$$F_{P,3} = 2F_{B,3} \qquad (2.2)$$

Again we need a system with borders that cross internal streams.

Draw system borders that enclose both separators.

Scheme II. Separate unreacted *A* from by-product *B* and recycle *A*.




Model 1: (3 streams) × (3 parameters/stream) = 9 parameters

Calculate the flow rates of streams 1 and 6, in kg/min. Calculate the flow rate and composition of stream 3.

Model 2: (4 streams) × (3 parameters/stream) = 12 parameters

# Model 2 of Scheme II – Mathematical Model

Write a mass balance on $P$ (note: no chemical reactions).

rate of $P$ in = rate of $P$ out

$$F_{P,3} = F_{P,4} + \cancelto{0}{F_{P,6}} + \cancelto{0}{F_{P,7}} \qquad \text{(informal)}$$

$$F_{P,3} = F_{P,4} \qquad (3.1)$$

Write a mass balance on $B$ (note: no chemical reactions).

rate of $B$ in = rate of $B$ out

$$F_{B,3} = \cancelto{0}{F_{B,4}} + F_{B,6} + \cancelto{0}{F_{B,7}} \qquad \text{(informal)}$$

$$F_{B,3} = F_{B,6} \qquad (3.2)$$

Substitute equations (3.1) and (3.2) into equation (2.2).

$$F_{P,3} = 2F_{B,3} \qquad (2.2)$$

$$F_{P,4} = 2F_{B,6} \qquad (3.3)$$

# Model 2 of Scheme II – Mathematical Model, cont'd

Substitute equation (6) ($F_{P,4}$ = 100 kg/min) into equation (3.3).

$$F_{P,4} = 2F_{B,6} \qquad (3.3)$$

$$100 = 2F_{B,6}$$

$$F_{B,6} = 50.\ \text{kg/min} \qquad (3.4)$$

Substitute equations (2)-(8) and (3.4) into the overall mass balance (equation 1).

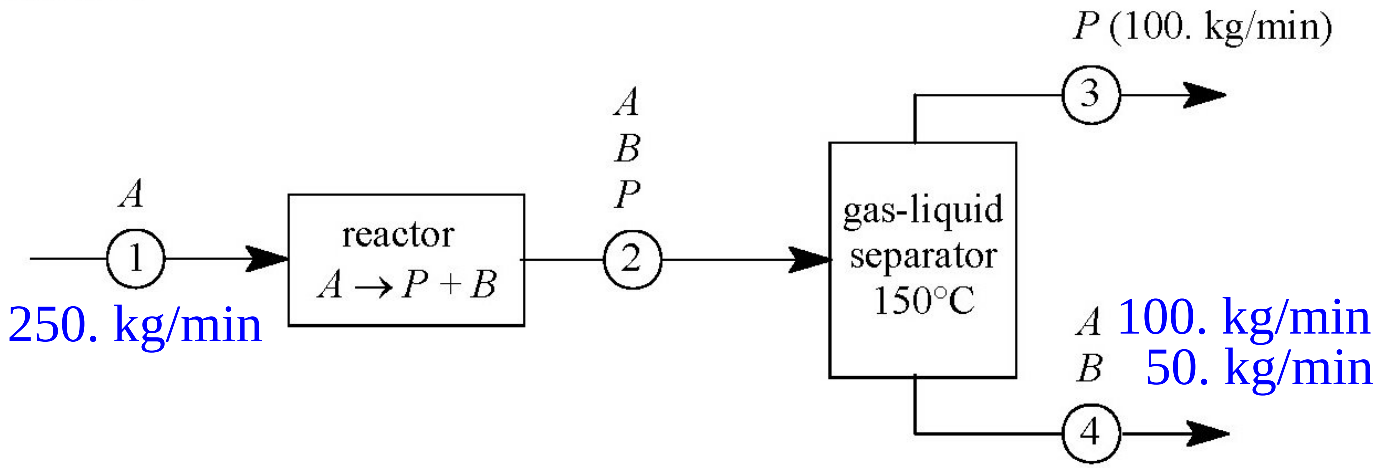
$$F_{P,1} + F_{A,1} + F_{B,1} = F_{P,4} + F_{P,6} + F_{A,4} + F_{A,6} + F_{B,4} + F_{B,6} \qquad (1)$$

$$0 + F_{A,1} + 0 = 100 + 0 + 0 + 0 + 0 + 50$$

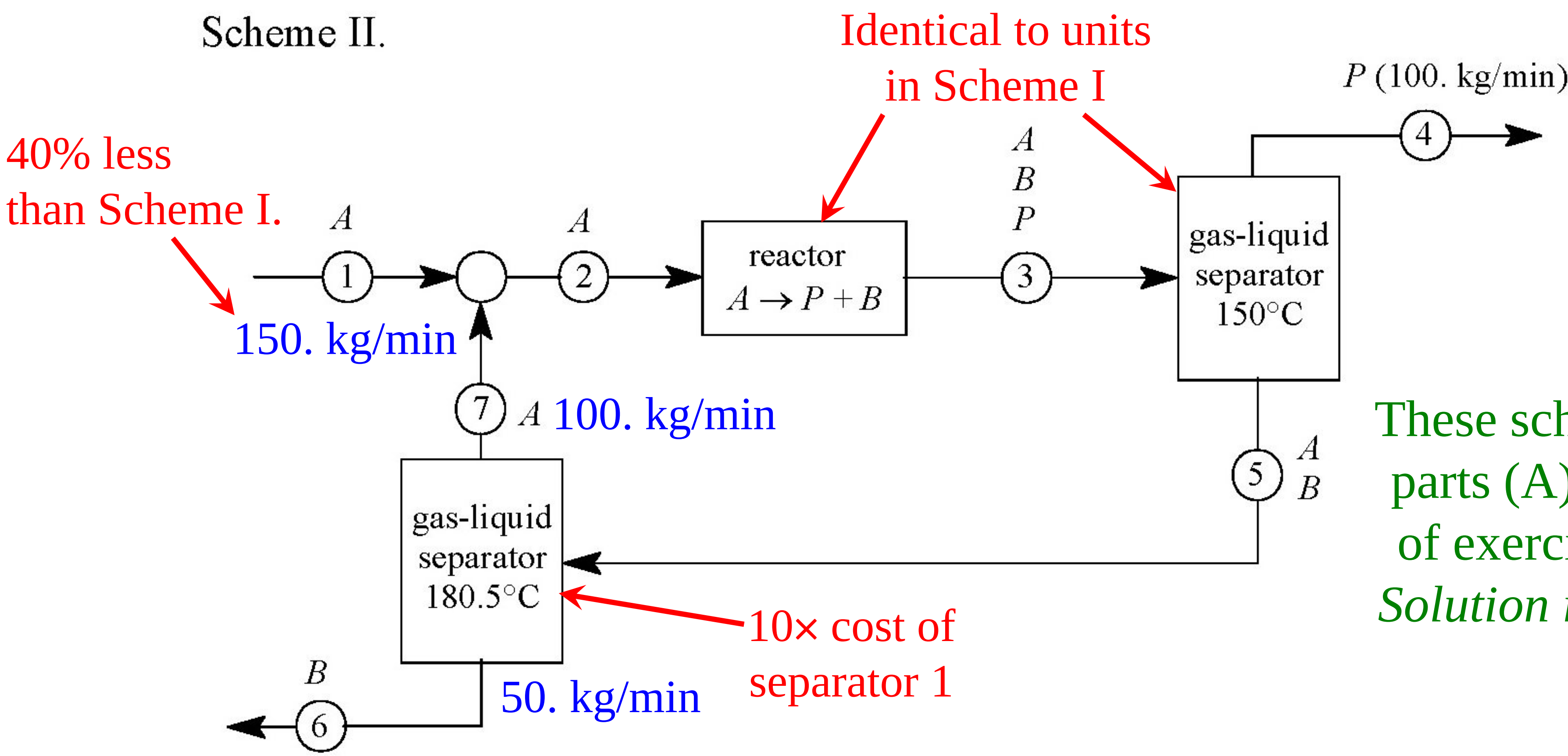
$$F_{A,1} = 150\ \text{kg/min}$$

# Summary of Schemes I and II.

Scheme I.




Scheme II.




These schemes are parts (A) and (B) of exercise 3.44. *Solution is posted.*