EngrD 2190 – Lecture 11

Concept: Process Analysis – Mathematical Modeling with
Energy Balances

- One cannot measure energy; one must use measurable quantities (temperature and phase) and convert to energy.
- One cannot calculate absolute energy; one must calculate energy *change*.

Context: A heater, a heater + partial evaporator,
and a heat exchanger.

Defining Question: What is an elementary energy process unit?

Read Chapter 3 pp. 123-132 (energy balances)

EngrD 2190 – Lecture 11

Homework 3 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 between 130 and 132 Olin Hall. **Not to my mailbox.**

EngrD 2190 – Lecture 11

- Homework 4 due Friday 9/26:

  Formal mass balances on processes with chemical reactions:
  exercises 3.33 and 3.43
  Append a list of 'take-aways' to each exercise.
  Every equation must have an explicit source.

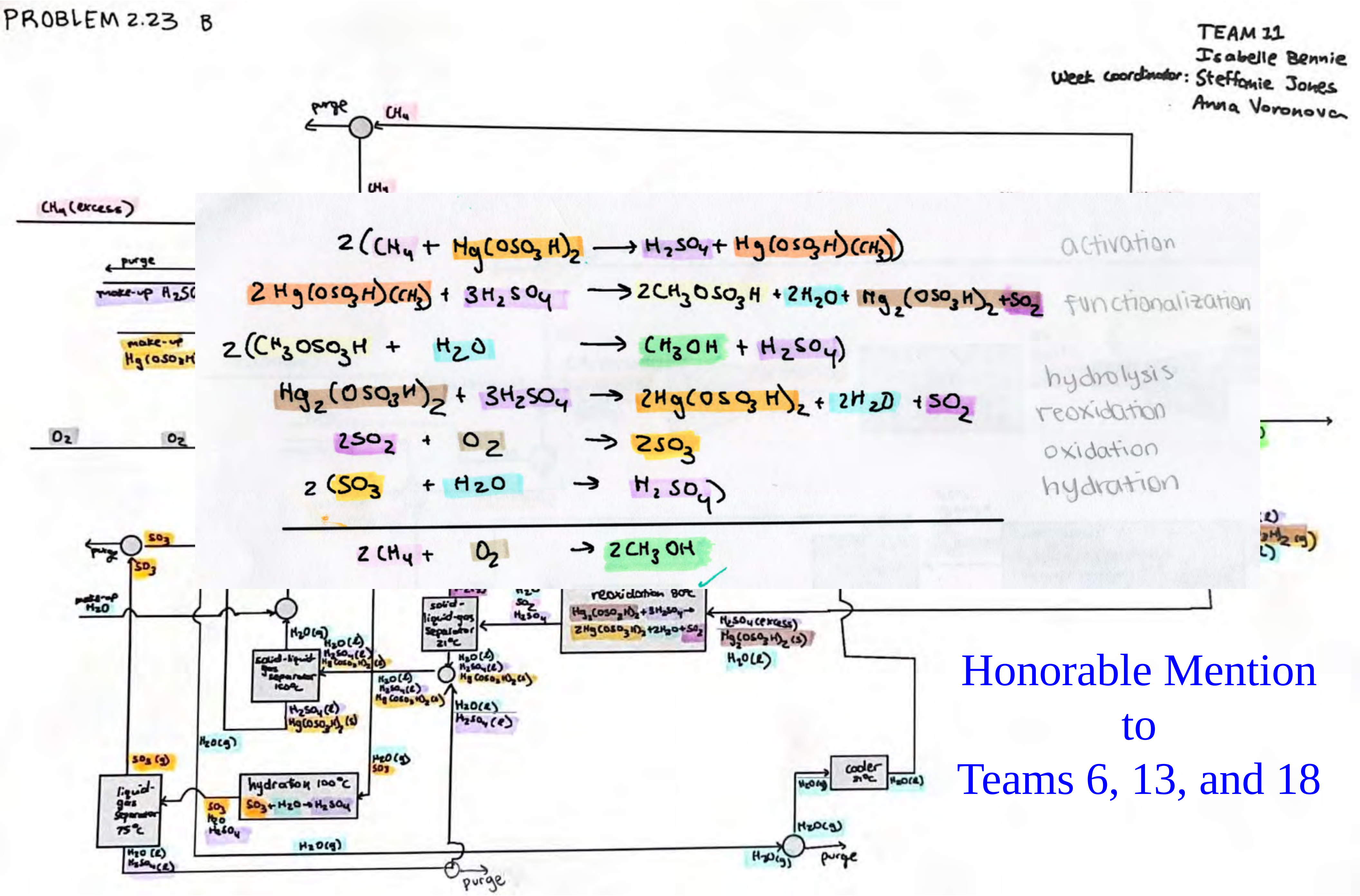
  Process Design with qualitative, informal mass balances:
  exercises 3.119 and 3.124
  Append a list of 'take-aways' to each exercise.

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.

Homework 2 Excellence – Exercise 2.23 – Team 11



PROBLEM 2.23 B

TEAM 11
Isabelle Bennie
Week coordinator: Steffanie Jones
Anna Voronova

$2(CH_4 + Hg(OSO_3H)_2 \longrightarrow H_2SO_4 + Hg(OSO_3H)(CH_3))$ activation

$2Hg(OSO_3H)(CH_3) + 3H_2SO_4 \longrightarrow 2CH_3OSO_3H + 2H_2O + Hg_2(OSO_3H)_2 + SO_2$ functionalization

$2(CH_3OSO_3H + H_2O \longrightarrow CH_3OH + H_2SO_4)$ hydrolysis

$Hg_2(OSO_3H)_2 + 3H_2SO_4 \longrightarrow 2Hg(OSO_3H)_2 + 2H_2O + SO_2$ reoxidation

$2SO_2 + O_2 \longrightarrow 2SO_3$ oxidation

$2(SO_3 + H_2O \rightarrow H_2SO_4)$ hydration

$2CH_4 + O_2 \rightarrow 2CH_3OH$ ✓

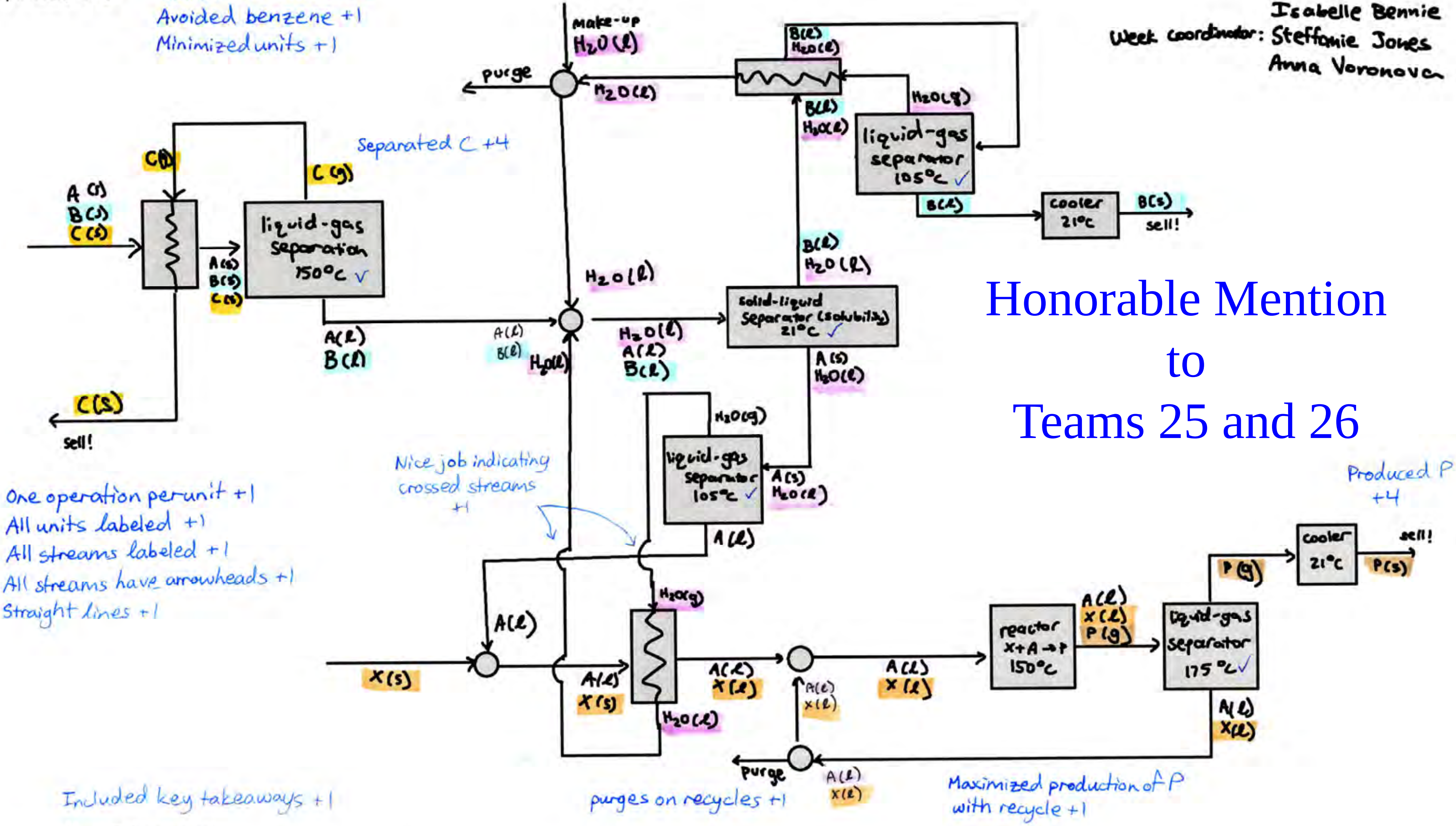
Honorable Mention
to
Teams 6, 13, and 18

Homework 2 Excellence – Exercise 2.33 – Team 11

PROBLEM 2.33

TEAM 11
Isabelle Bennie
Week coordinator: Steffonie Jones
Anna Voronova

Correct separator temperatures +3
Used heat exchangers to minimize wasted energy +1
No material waste +2
Avoided benzene +1
Minimized units +1



Separated C +4

Nice job indicating crossed streams +1

One operation per unit +1
All units labeled +1
All streams labeled +1
All streams have arrowheads +1
Straight lines +1

Produced P +4

Included key takeaways +1

purges on recycles +1

Maximized production of P with recycle +1

Honorable Mention
to
Teams 25 and 26

Key Takeaways:
1. Heat exchangers can greatly reduce the amount of energy needed for a process
2. It is easiest to sell solids.
3. Solubility separators can be useful when liquid-gas seperators are not feasible or more energetically taxing.

Mathematical Modeling

Translate a physical and chemical description into equations.

Part 1. Mass Balances

must define system borders

Universal Laws

Conservation of Mass $F_{\mathrm{T,in}} = F_{\mathrm{T,out}}$

Process Specifications

5% of the recycle is purged ⇒ $0.05 \times F_{\mathrm{T,recycle}} = F_{\mathrm{T,purge}}$

× =

Part 2. Energy Balances

Universal Laws

Conservation of Energy $q_{\mathrm{in}} = q_{\mathrm{out}}$

Constitutive ‘Laws’

$$\left.\begin{aligned} \Delta q &= F_{\mathrm{T}} C_{\mathrm{P}} (T_{\mathrm{out}} - T_{\mathrm{in}}) \\ \Delta q &= F_{\mathrm{T}} (\Delta H_{\mathrm{phase}}) \end{aligned}\right\}$$

from classical thermodynamics

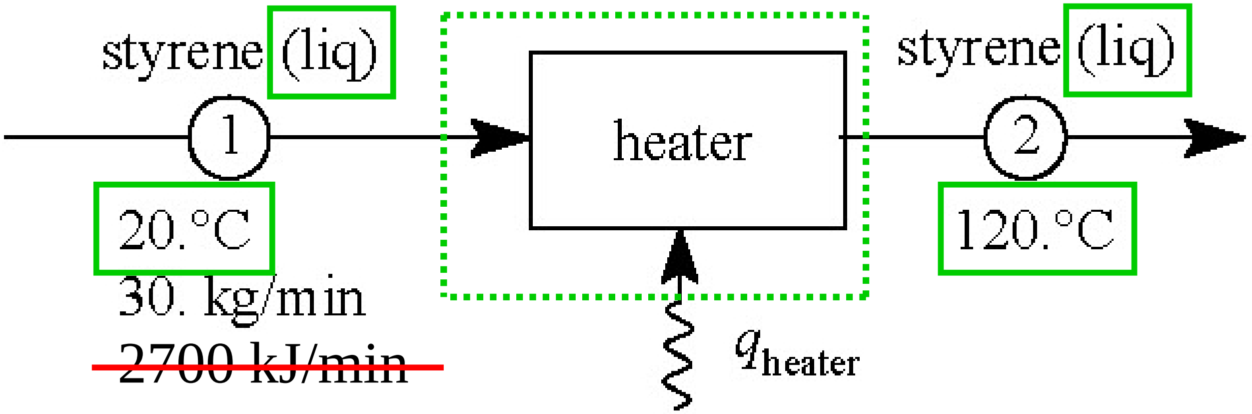
phenomenological; from empirical relations, not from basic principles

Part 3. $ Balances

Energy Balance Example 1

Example 1. Calculate q_{heater}.

energy indicators: phase and temperature



Cannot specify absolute energy flow rates.
Can only specify *differences* between energy flow rates.

Cannot measure differences between energy flow rates.
Must measure energy indicators and calculate energy differences.

Applying an Energy Balance

Define $q_i \equiv$ flow rate of energy in stream *i* (kJ/min)

Apply the Conservation of Energy

Shorthand for
1. steady state (in = out)
2. system with green borders

rate of energy in = rate of energy out

$$q_1 + q_{\text{heater}} = q_2$$

$q_1 = ?$ Use an 'energy meter' on stream 1? No. Does not exist.

We can measure the mass of a stream,
but we cannot measure the energy of a stream.

Must use energy indicators. Temperature!

How to convert *T* to *q*? Thermodynamics!

(change in internal energy) $\propto$ (mass) × (change in temperature) for $\Delta P = 0$

$$\Delta U = (\text{mass}) \times C_P \times \Delta T$$

proportionality constant – heat capacity

"constant" is not constant – changes with substance
– changes with *T* and *P*

Applying an Energy Balance, cont’d

$$\Delta U \;=\; (\text{mass}) \times C_{\text{P}} \times \Delta T$$

Divide both sides by time $$\frac{\Delta U}{\text{time}} \;=\; \frac{\text{mass}}{\text{time}} \times \overline{C}_{\text{P}} \times \Delta T$$

$$\Delta q \;=\; F\,\overline{C}_{\text{P}}\,(\Delta T)$$ equation 3.114

Note: we do *not* have an equation for $q = \ldots$ We must group q’s into Δq’s

Return to the energy balance on the heater.

rate of energy in = rate of energy out

$$q_1 \;+\; q_{\text{heater}} \;=\; q_2$$

Group q’s into connected mass streams:

$$q_{\text{heater}} \;=\; \underbrace{q_2 - q_1} = \;\Delta q_{1\rightarrow 2}$$

streams 1 and 2 are same substance: styrene

streams 1 and 2 have same flow rate: 100 kg/min

q difference arranged as ‘out’ minus ‘in’

Applying an Energy Balance, cont'd

$$q_{\text{heater}} = \Delta q_{1\to 2}$$

Use thermodynamics to substitute for Δq.

$$q_{\text{heater}} = F_{\text{T},1}\overline{C}_{\text{P,styrene}}(T_2 - T_1)$$

assumes C_{P} is independent of T

Calculate a numerical value. *Include explicit units.*

see data on p. 200

$$q_{\text{heater}} = \left(\frac{30\ \cancel{\text{kg styrene}}}{\text{min}}\right)\left(\frac{183\text{ joules}}{{}^{\text{o}}\cancel{\text{C}}\cdot\cancel{\text{mol }\underline{\text{styrene}}}}\right)(120^{\text{o}}\cancel{\text{C}} - 20^{\text{o}}\cancel{\text{C}})\left(\frac{1\ \cancel{\text{mol styrene}}}{104\ \cancel{\text{g styrene}}}\right)\left(\frac{\cancel{1000\text{ g}}}{\cancel{1\text{ kg}}}\right)$$

important

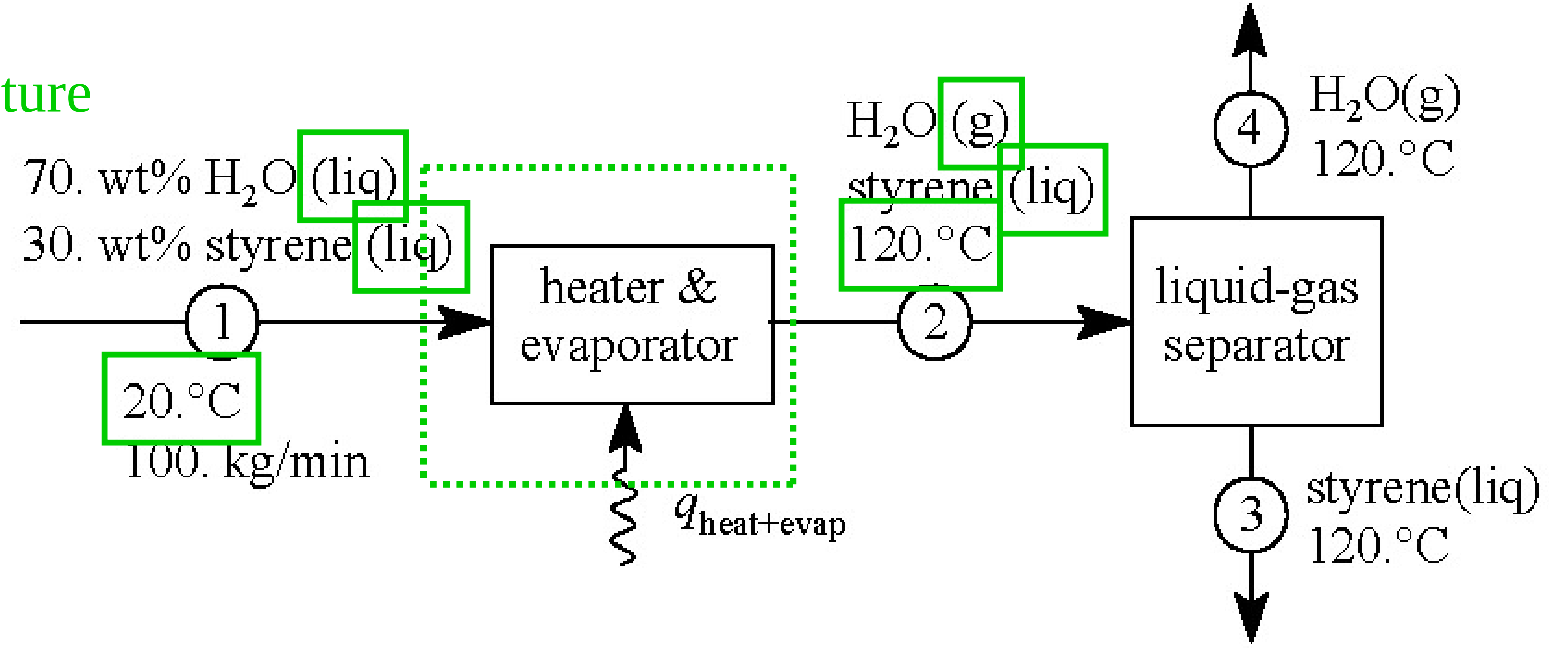
$$q_{\text{heater}} = 5.279 \times 10^{6}\text{ joules/min}$$

$$\boxed{q_{\text{heater}} = 5.3 \times 10^{3}\text{ kJ/min}}$$

Energy Balance Example 2

Example 2: Exercise 3.63(A). Calculate $q_{\text{heat+evap}}$. *Solution is posted.*

energy indicators:
phase and temperature



Although the mass balance is simple, the energy balance is complicated.

Heat styrene (liquid) to 120°C.

Heat water (liquid) to 100°C.

Evaporate water (liquid) at 100°C.

Heat steam (vapor) to 120°C.

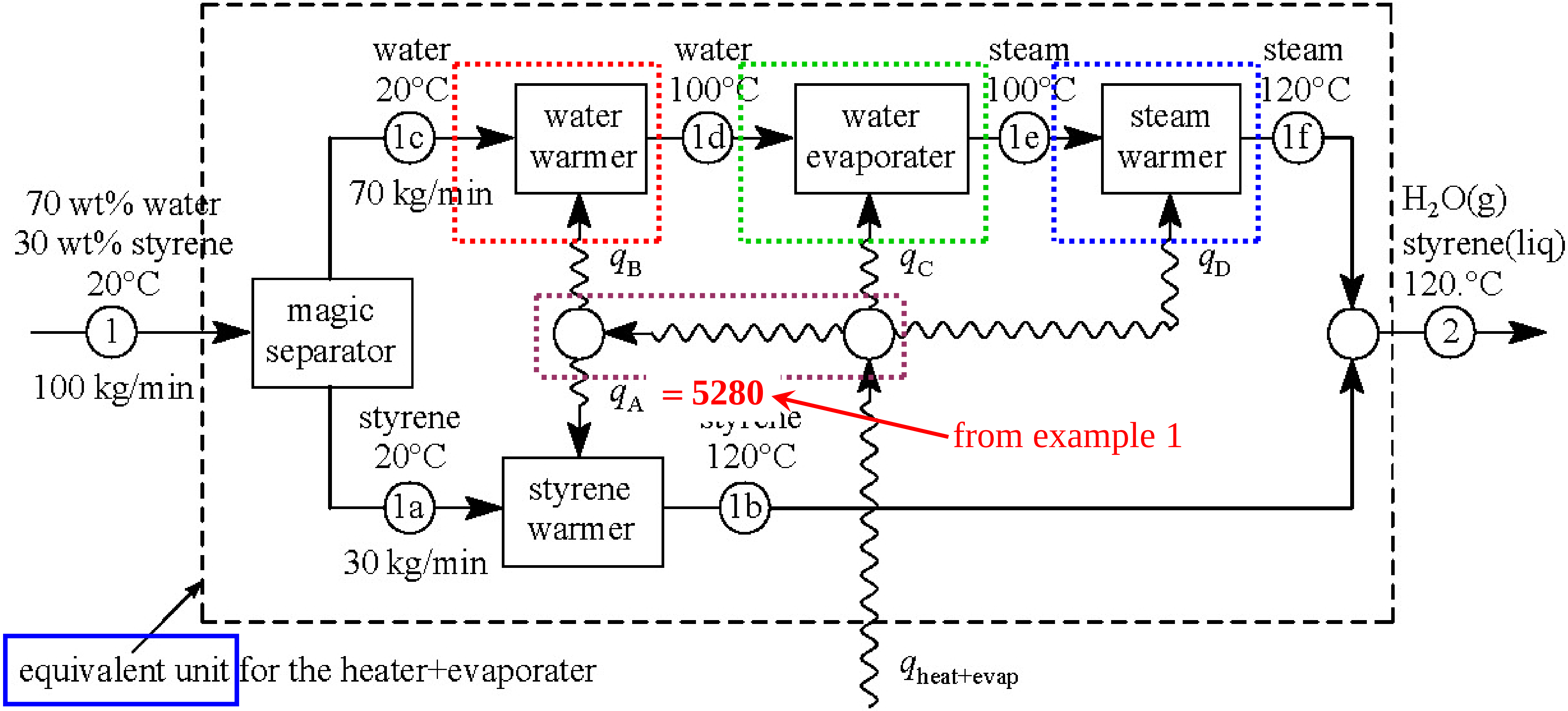
Strategy: represent heater+evaporator as a system of elementary energy units.

one mass stream in, one mass stream out

one energy change: temperature change
or phase change
or pressure change
or velocity change …

in later courses

Example 2: Exercise 3.63(A). Equivalent unit for heater+evaporator:



Comprises *elementary* energy units

- one stream in, one stream out.
- one energy change: ΔT or Δphase (EngrD 2190)
  ΔP, Δv, Δheight, etc (later courses)

Example 2: Energy Balance on Heater+Evaporator

Water warmer: rate of energy in = rate of energy out

$$q_{1c} + q_B = q_{1d}$$

Group q’s into Δq’s: $q_B = q_{1d} - q_{1c} = F_{T,1c}\overline{C}_{P,\text{water}}(T_{1d} - T_{1c})$

$$q_B = \left(\frac{70\text{ kg water}}{\text{min}}\right)\left(\frac{75\text{ joules}}{{}^{\text{o}}\text{C}\cdot\text{mol water}}\right)(100-20^{\text{o}}\,\text{C})\left(\frac{1000\text{ mol water}}{18\text{ kg water}}\right)$$

$$q_B = 23{,}350\text{ kJ/min}$$

Evaporator: rate of energy in = rate of energy out

$$q_{1d} + q_C = q_{1e}$$

Group q’s into Δq’s: $q_C = q_{1e} - q_{1d} = \xcancel{F_{T,1d}\overline{C}_{P,\text{water}}(T_{1e} - T_{1d})}$

$$= F_{T,1d}\Delta\overline{H}_{\text{vaporization}}$$

$$q_C = \left(\frac{70\text{ kg water}}{\text{min}}\right)\left(\frac{4.1\times10^4\text{ joules}}{\text{mol water}}\right)\left(\frac{1000\text{ mol water}}{18\text{ kg water}}\right)$$

$$q_C = 159{,}600\text{ kJ/min}$$

Example 2: Energy Balance on Heater+Evaporator, cont'd

Steam warmer: rate of energy in = rate of energy out

$$q_{1e} + q_D = q_{1f}$$

Group q's into Δq's: $q_D = q_{1f} - q_{1e} = F_{T,1e} C_{P,steam}(T_{1f} - T_{1e})$

$$q_D = \left(\frac{70 \text{ kg steam}}{\text{min}}\right)\left(\frac{35 \text{ joules}}{{}^{o}\text{C} \cdot \text{mol steam}}\right)(120 - 100^{o}\text{C})\left(\frac{1000 \text{ mol steam}}{18 \text{ kg steam}}\right)$$

$$q_D = 2720 \text{ kJ/min}$$

Combine the energy flows to the elementary energy units.

Write an energy balance on a fictitious energy combiner.

rate of energy in = rate of energy out

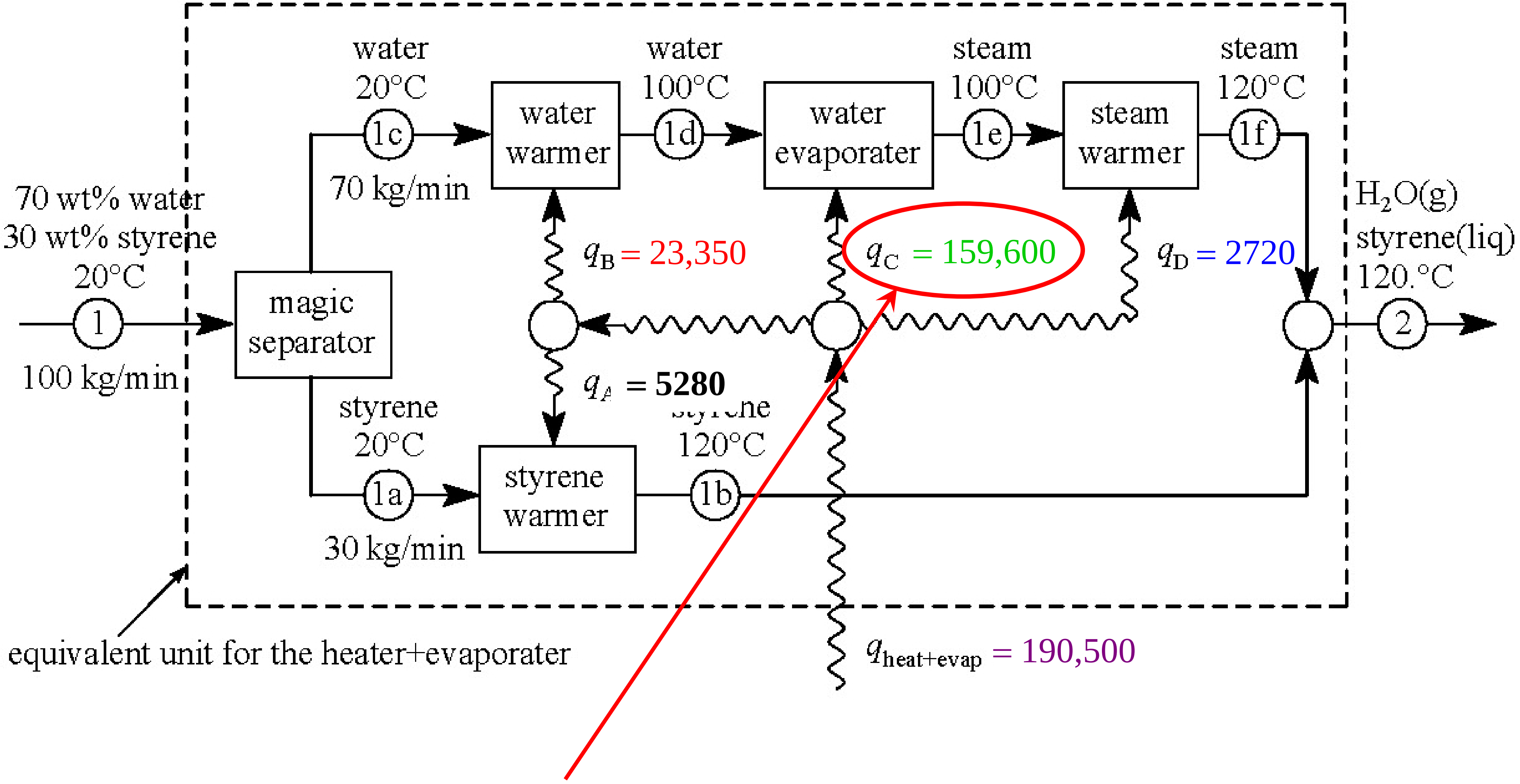
$$q_{\text{heater+evaporator}} = q_A + q_B + q_C + q_D$$

$$q_{\text{heater+evaporator}} = 5280 + 23{,}350 + 159{,}600 + 2720$$

$$q_{\text{heater+evaporator}} = 190{,}950 \text{ kJ/min}$$

$$\boxed{q_{\text{heater+evaporator}} = 1.91 \times 10^5 \text{ kJ/min}}$$

Example 2: Exercise 3.63(A). Equivalent unit for heater+evaporator:



Important: evaporating the water is the major energy use.

Best source of energy to recover in a heat exchanger (Example 3)

Defining Question: What is an elementary energy process unit?

Answer: An elementary energy process unit is a fictitious unit to
represent a single energy change for a single mass stream.

An elementary energy process unit has –
one stream in and one stream out, and
exactly one energy change – a temperature change, or
a phase change, or
in later courses ↓ a velocity change, or
a pressure change, or
a height change, or …

Replace a complex energy unit with an Equivalent Unit that comprises elementary energy process units.

Bring Today’s Lecture Handout to Monday’s Lecture.