# EngrD 2190 – Lecture 34

# Course Summary and Review – Part 1
# Mathematical Modeling

## Final Exam

Friday, December 12, 7:00 - 9:30 p.m., 128 and 245 Olin Hall.

Comprehensive - covers chapters 2 through 5, with emphasis on chapter 5: dimensional analysis and dynamic scaling.

Open notes and open exercise solutions.

Bring a calculator and a ruler/straightedge.

Graphing calculators are okay.

Applications for Affiliation are due Saturday December 20

Cornell Engineering

# Application For Major Affiliation

## Student Completes This Section

Last Name: ______________ First Name: ____________ Expected Degree Date: ________

NetID: ______________ ID# (7-digit): __________ Cell Phone: ____________

Major: ________________________________________
*(to which you are applying)*

Concentration/Interest within major: ______________________________
*(Optional, and if known)*

Current Advisor Name & Dept.: ______________________________

Student Signature: ______________________________ Date: __________

## After completing the top section, please submit to the Undergraduate Coordinator's office of the appropriate Major listed below:

**Biological Engineering (207 Riley-Robb Hall)**
**Biomedical Engineering (121 Weill Hall)***
**Chemical Engineering (158B Olin Hall)**
**Civil Engineering (221 Hollister Hall)**
**Computer Science (110 Gates Hall)***
**Earth and Atmospheric Sciences (2124 Snee Hall)**
**Electrical and Computer Engineering (222 Phillips Hall)**
**Environmental Engineering (221 Hollister Hall)**
**Engineering Physics (261 Clark Hall)**
**Information Science, System, and Tech (110H Gates Hall)***
**Materials Science and Engineering (210A Bard Hall)**
**Mechanical Engineering (125 Upson Hall)**
**Operations Research and Engineering (203 Rhodes Hall)**

*An additional application beyond this form is needed. Please see appropriate major for more information.

## Undergraduate Coordinator Completes This Section

Date Received: ______________________

Affiliation Approved ☐ Affiliation Conditional ☐ Affiliation Denied ☐

Conditions/Comments: ______________________________

______________________________

______________________________

Update Class/Term *(if needed)*: New Class (2,3,4): __________ New Term (1,2): __________

New Advisor: ______________ EMPL ID: __________ E-mail: __________

Authorizing Signature: ______________________________ Date: __________

**TYPICAL CURRICULUM in CHEMICAL & BIOMOLECULAR ENGINEERING**

**for a student with no advanced placement credits (class of 2025 and thereafter)**

| Semester 1 | | Semester 2 | |
|---|---|---|---|
| Math 1910 | 4 | Math 1920 | 4 |
| Chem 2090 | 4 | Phys 1112 | 4 |
| EngrI/ChemE 1120 | 3 | Chem 2080 (Approved Elective) | 4 |
| Freshman Writing Seminar | 3 | CS 1112 | 4 |
| | 14 | Freshman Writing Seminar | 3 |
| | | | 19 |

| Semester 3 | | Semester 4 | |
|---|---|---|---|
| Math 2930 | 4 | Math 2940/CEE 3040/EngrD 2700 | 4 |
| Phys 2213 | 4 | Chem 2900 (Major) | 2 |
| EngrD/ChemE 2190 | 4 | ChemE 2200 (Major) | 4 |
| Chem 3890 (EngrD Distribution) | 4 | ChemE 3230 (Major) | 4 |
| Liberal Studies Distribution | 3 | Liberal Studies Distribution | 3 |
| | | | 17 |

If you are on the ChemE track, you must complete ***both*** ChemE 2200 and ChemE 3230 in the 4th semester.

| Semester 5 | | | |
|---|---|---|---|
| ChemE 313 | | | 1 |
| ChemE 324 | | | 4 |
| Chem 3570 | | | 2 |
| Chem 2510 | | | 4 |
| Biology Elective** | 3 | Major-Approved Elective*** | 3 |
| Liberal Studies Distribution | 3 | Liberal Studies Distribution | 3 |
| | | | 17 |

You must complete ChemE 2200 – Physical Chemistry II for Engineers, not Chem 3900 – Honors Physical Chemistry II.

| Semeste | | | |
|---|---|---|---|
| ChemE | | | 4 |
| Advance | | | 3 |
| Major-A | | | 3 |
| Major-Approved Elective*** | 3 | Approved Elective | 3 |
| Liberal Studies Distribution | 3 | | 13 |
| | 16 | | |

# December 2025

| Sun | Mon | Tue | Wed | Thu | Fri | Sat |
|---|---|---|---|---|---|---|
| | 1 | 2 | 3<br>We are here | 4 | 5 | 6 |
| 7 | 8<br>TMD Office Hours noon – 2 p.m. | 9 | 10<br>TA Office Hours 2-4 p.m. | 11<br>TA Office Hours 2-4 p.m. | 12<br>EngrD 2190 7 p.m. | 13 |
| 14 | 15<br>Math 2930 2 p.m. | 16<br>Phys 2213 9 a.m. | 17<br>Math 2940 9 a.m. | 18 | 19<br>Chem 3890 7 p.m. | 20 |
| 21 | 22 | 23 | 24 | 25 | 26 | 27 |
| 28 | 29 | 30 | 31 | | | |

# EngrD 2190 – Chemical Process Design & Analysis

## Course Summary and Review – Part 1

## Mathematical Modeling

| week | date | | lecture | dates | calculation session |
|---|---|---|---|---|---|
| 1 | 8/25 | 1 | course content, course objectives, and course organization.<br>reading: chapter 1, pp. 1-7, chapter 2, pp. 8-19. | | |
| | 8/27 | 2 | Concept: process design - unit operations and process flowsheets.<br>Context: green chemistry for hydrazine synthesis.<br>reading: chapter 2, pp 20-25. | CS 1<br>8/27 | process analysis & design by incremental evolution.<br>exercises 2.9 and 2.22. |
| | 8/29 | 3 | Concept: process design - problem solving<br>Context: strategies for separation - purification of $Br_2$<br>reading: chapter 2, pp 25-42.<br>homework 1: exercises 2.7, 2.24, and 2.25(A). | | |
| 2 | 9/1 | | *Labor Day - no lecture* | | |
| | 9/3 | 4 | Concept: process design - devising chemical cycles.<br>Context: producing $CH_4$ from $CO_2$ and thermal energy.<br>reading: chapter 2, pp 42-48. | CS 2<br>9/3 | problem redefinition: exercises 2.45, 2.38, and 2.40.<br>process analysis & design by incremental evolution: exercises 2.34 and 2.32.<br>professional development - part 1: résumés |
| | 9/5 | 5 | Concept: process design - reactors for solid reactants and products; reactants in excess to simplify separations.<br>Context: $CH_4$ from $CO_2$ and thermal energy, cont'd.<br>homework 2: exercises 2.23, 2.33, 2.43, 2.46, and 2.52. | | |
| 3 | 9/8 | 6 | Concept: process design - design evolution by incremental improvement.<br>Context: example exercises with approximate flow rates.<br>reading: chapter 3, pp. 89-99 and appendix C. | | |
| | 9/10 | 7 | Concept: process analysis - mathematical modeling based on fundamental laws.<br>Context: mass balances on processes without chemical reaction.<br>reading: chapter 3, pp. 99-106. | CS 3<br>9/10 | process analysis & design by incremental evolution: exercise 2.35.<br>process design and process analysis with mass balances: exercises 3.4 and 3.10.<br>professional development - part 2: elevator pitches |
| | 9/12 | 8 | Concept: mathematical modeling - mass balances.<br>Context: processes with chemical reactions - options for unreacted reactants.<br>reading: chapter 3, pp. 106-110.<br>homework 3: exercises 3.12, 3.28, 3.115, and 3.125. | | |
| 4 | 9/15 | 9 | Concept: mathematical modeling - mass balances<br>Context: options for unreacted reactants, cont'd.<br>reading: chapter 3, pp. 110-117. | | |
| | 9/17 | 10 | Concept: mathematical modeling - mass balances<br>Context: informal mass balances - estimating flow rates.<br>reading: chapter 3, pp. 117-123. | CS 4<br>9/17 | process analysis - informal mass balances for design: exercises 2.34 redux, 3.116, and 3.114. |
| | 9/19 | 11 | Concept: mathematical modeling - energy balances.<br>Context: heaters and heat exchangers.<br>reading: chapter 3, pp. 123-132.<br>homework 4: exercises 3.33, 3.43, 3.119, and 3.124. | | |
| 5 | 9/22 | 12 | Concept: mathematical modeling - energy balances.<br>Context: modeling a complex unit as several simple units.<br>reading: chapter 3, pp. 132-139. | | |

Homework, Calculation Sessions, and Exams - 108 exercises!

Practice exercises for mathematical energy balances: 3.69 and 3.75. Solutions are posted.

Chemical engineers create

processes and products

based on

chemical change.

chemical and biochemical change.

A process is divided into unit operations, represented by a process flowsheet.

How to create a process?

# Course Objectives

*Overall*

To introduce basic principles of engineering design and analysis in the context of chemical and biomolecular engineering.

*Engineering Skills*

To design a chemical and biomolecular process by the following steps:

- define the *real* problem
- generate ideas.
- create a design.
- analyze the design.

$$A + B \rightarrow P$$

Problem: Deliver $A$ and $B$ to a reactor.

*Real* Problem: Produce $P$.

To analyze a chemical and biomolecular process with three methods:

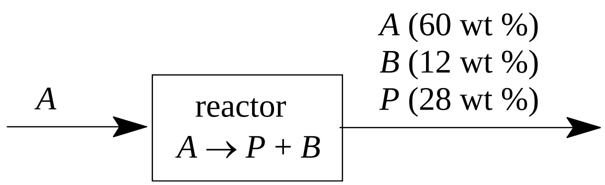
- mathematical modeling.
- graphical modeling.
- dimensional analysis & dynamic scaling

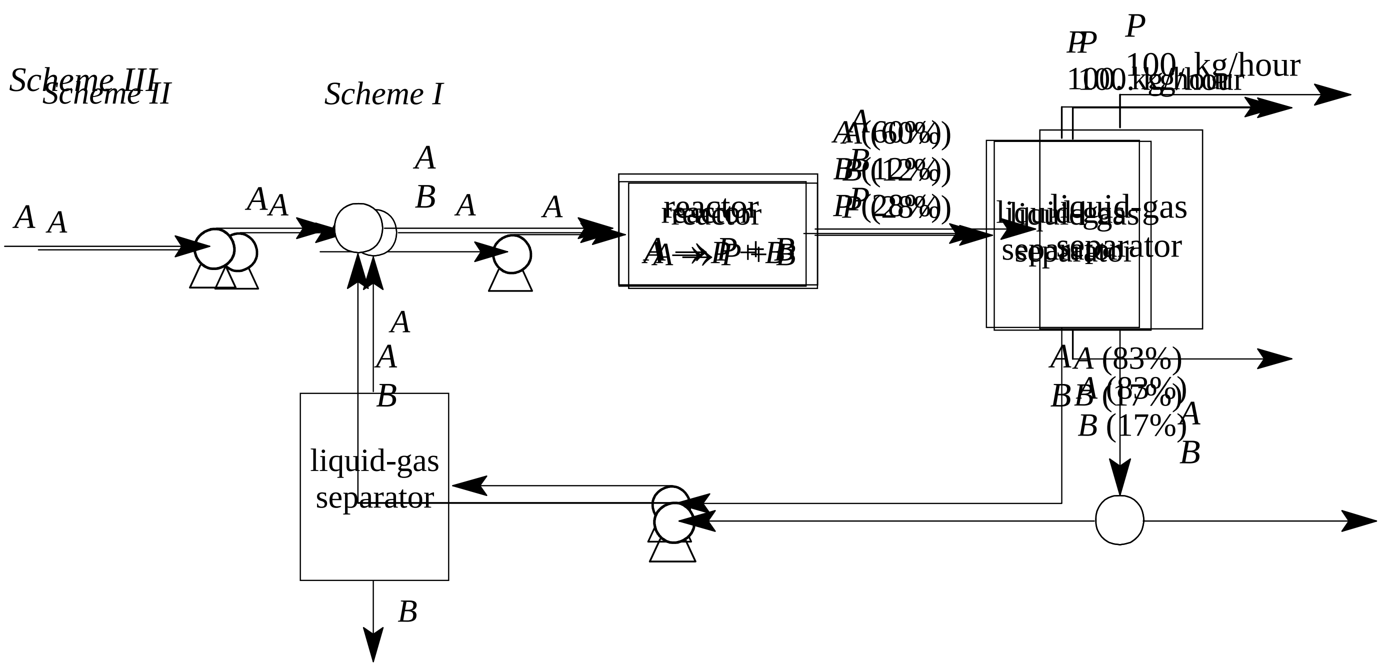
# Mathematical Modeling

Reactant *A* decomposes to *P* (product) and *B* (by-product).

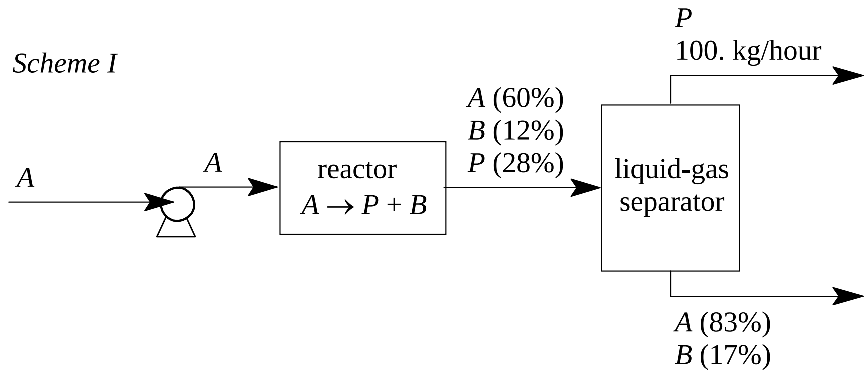
$$A \rightarrow P + B$$

The molecular weight ratio of *P* to *B* is 7:3, so 10 kg of *A* reacts to form 7 kg of *P* and 3 kg of *B*. The reactor converts 40% of *A*.

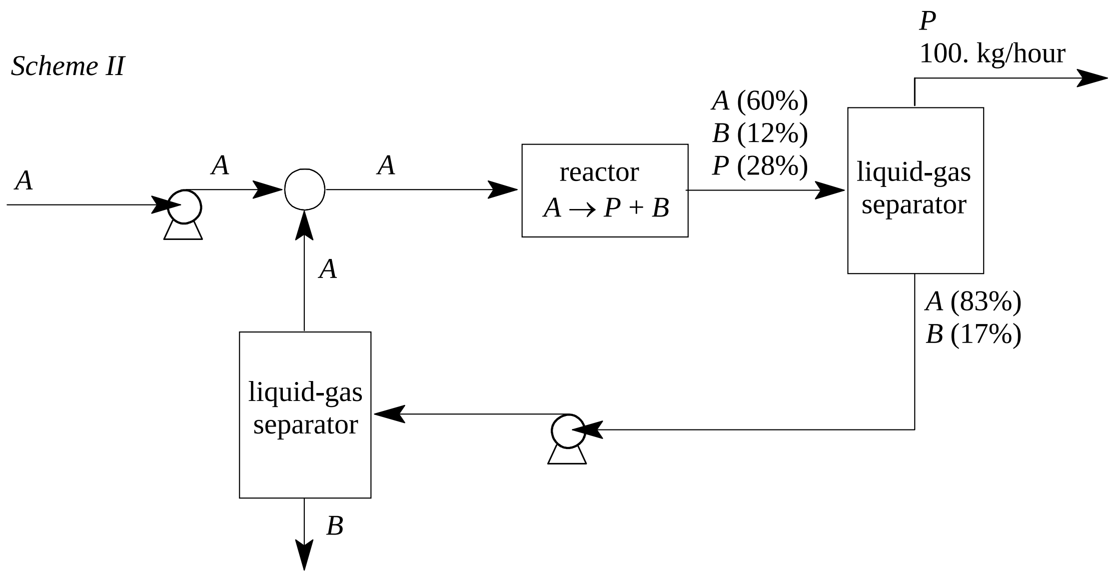


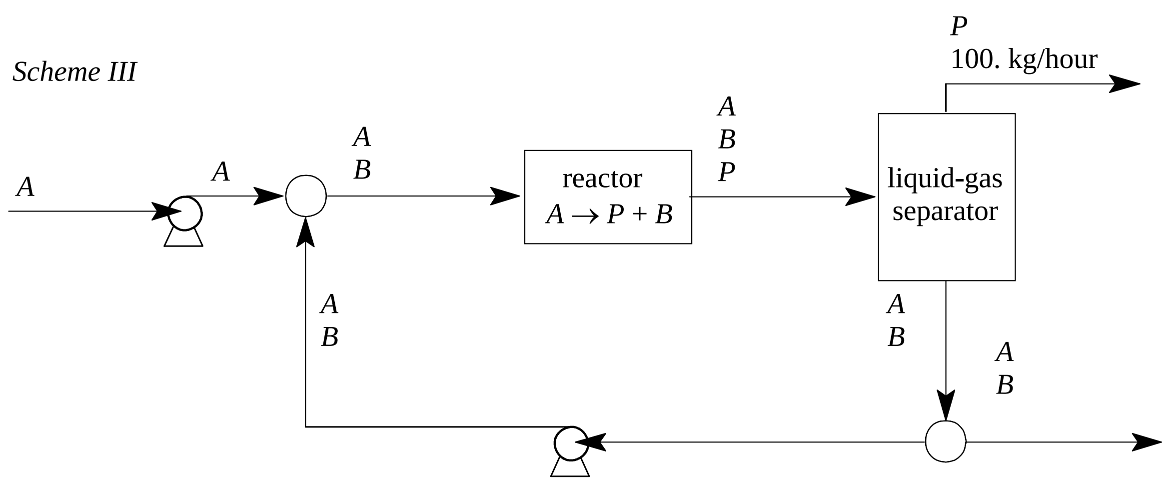
*Scheme I*




*Scheme II*




*Scheme III*




# Which to build?
# How to compare?

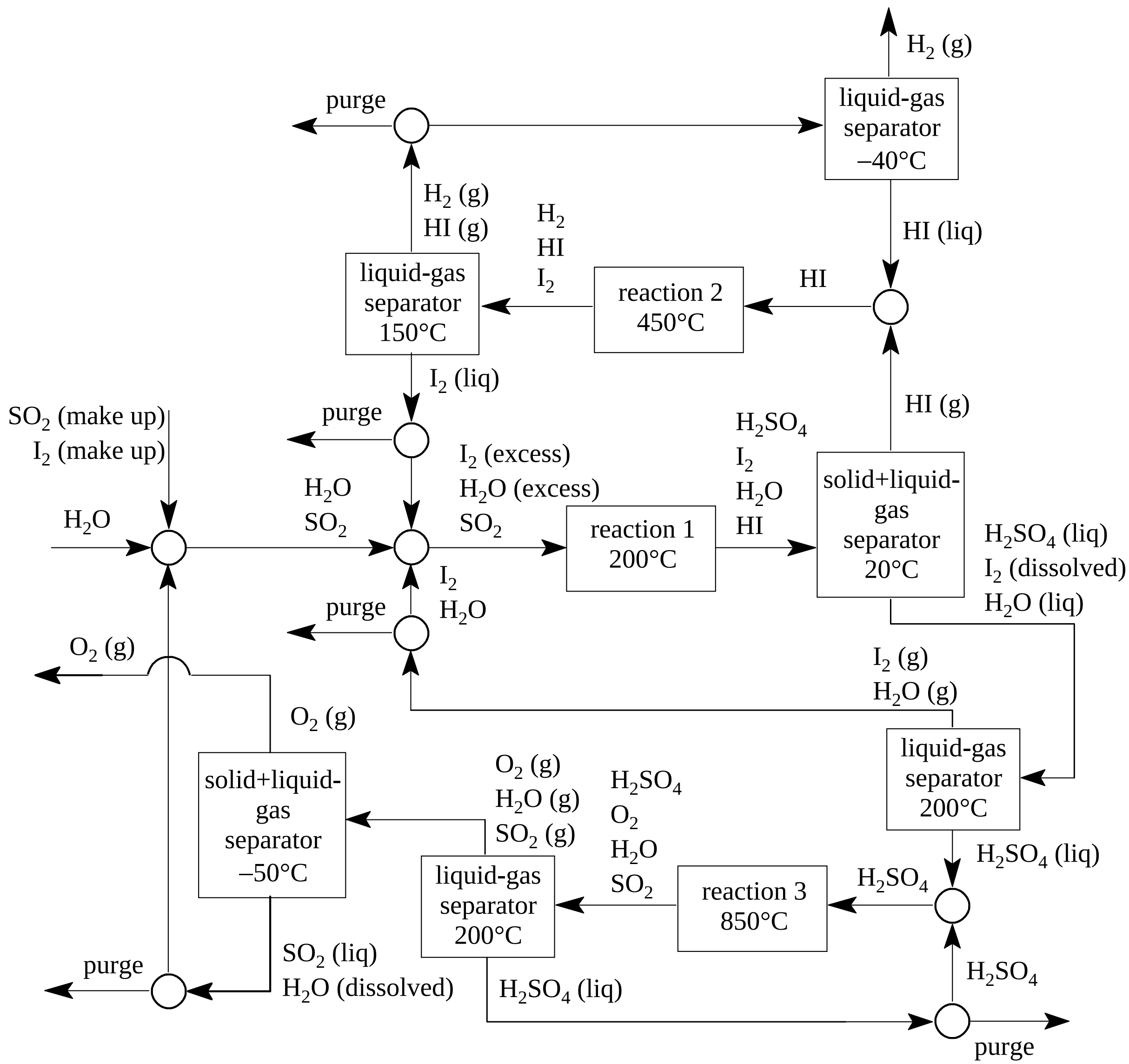
# Mass flow rates

# Energy flow rates

# Asset flow rates

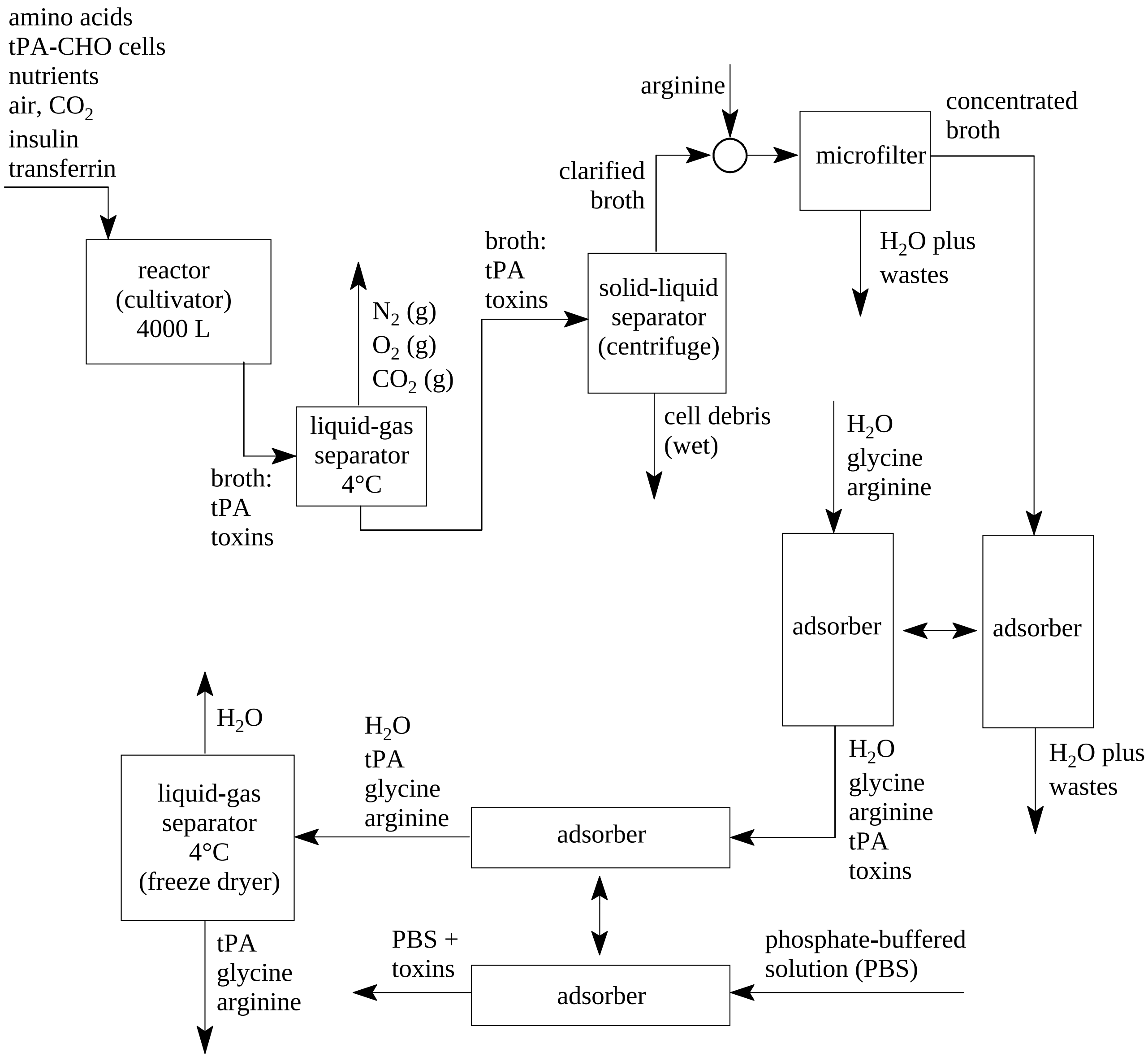
# Hydrogen Fuel from Thermal Energy

Overall Reaction: $H_2O \rightarrow H_2 + ½O_2$

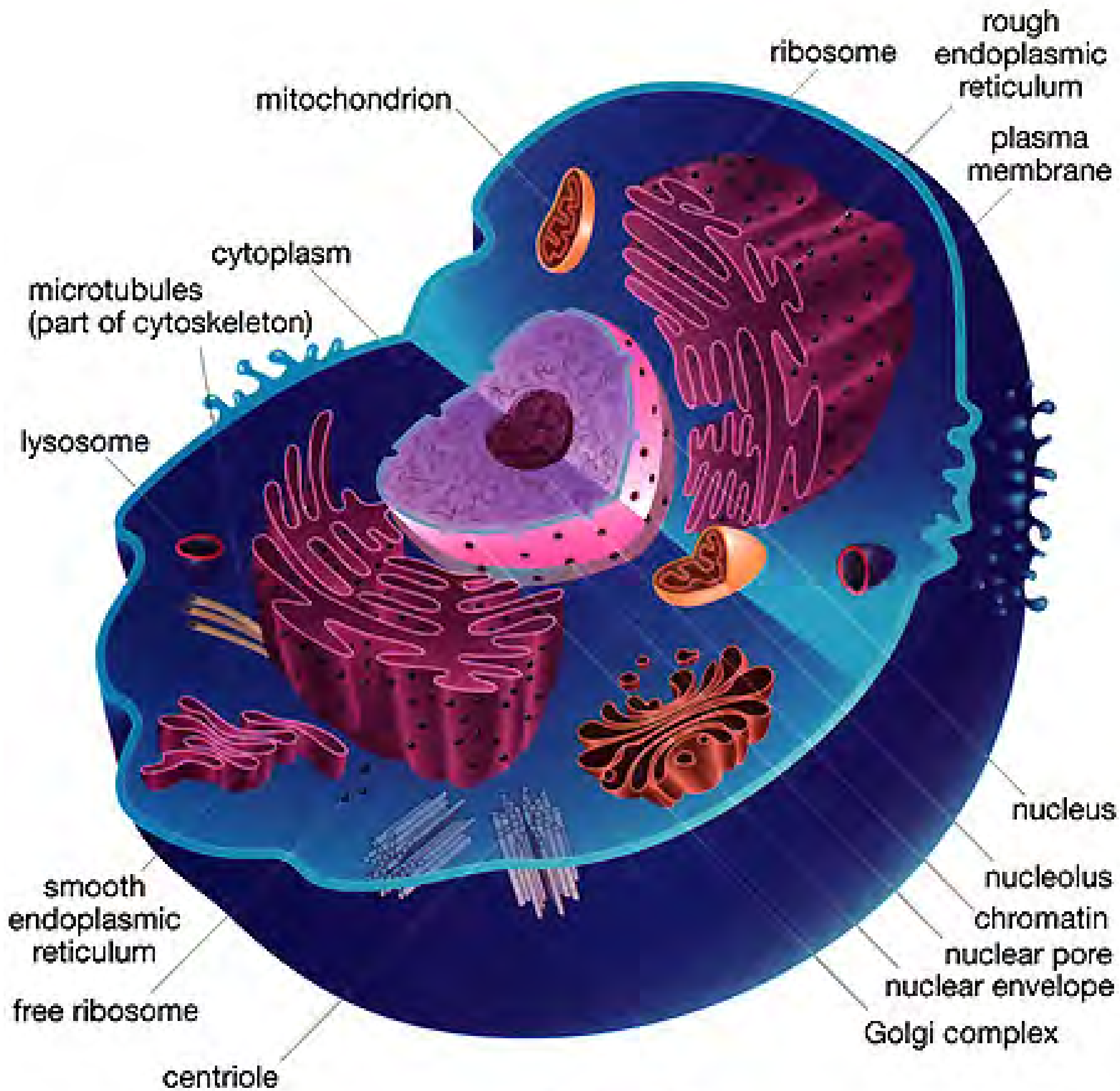


# Manufacturing Human Tissue Plasminogen Activator (tPA)

## Overall Reaction: 532 amino acids $\rightarrow$ tPA

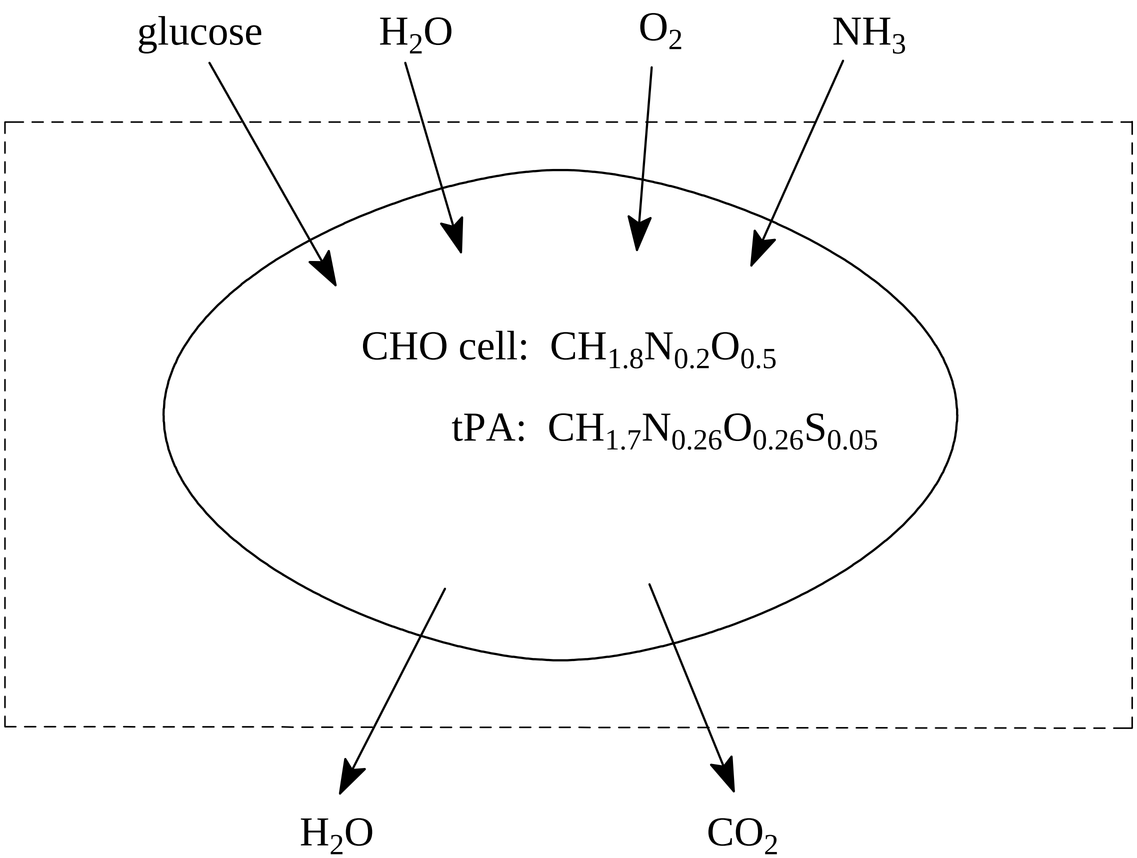


# The Cell as a Chemical Process

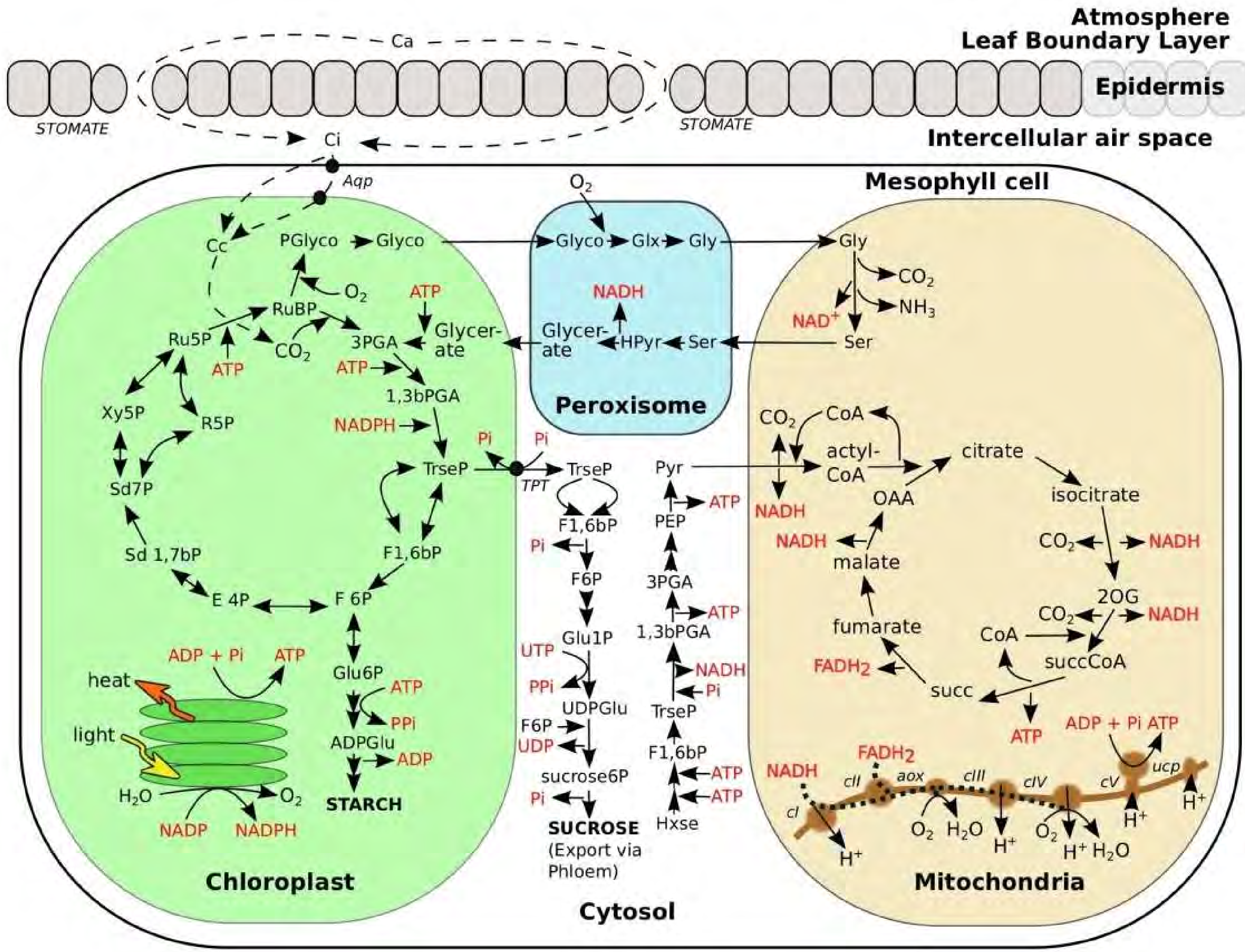



BIOLOGY: Life on Earth, Fifth Edition
by Teresa Audesirk and Gerald Audesirk

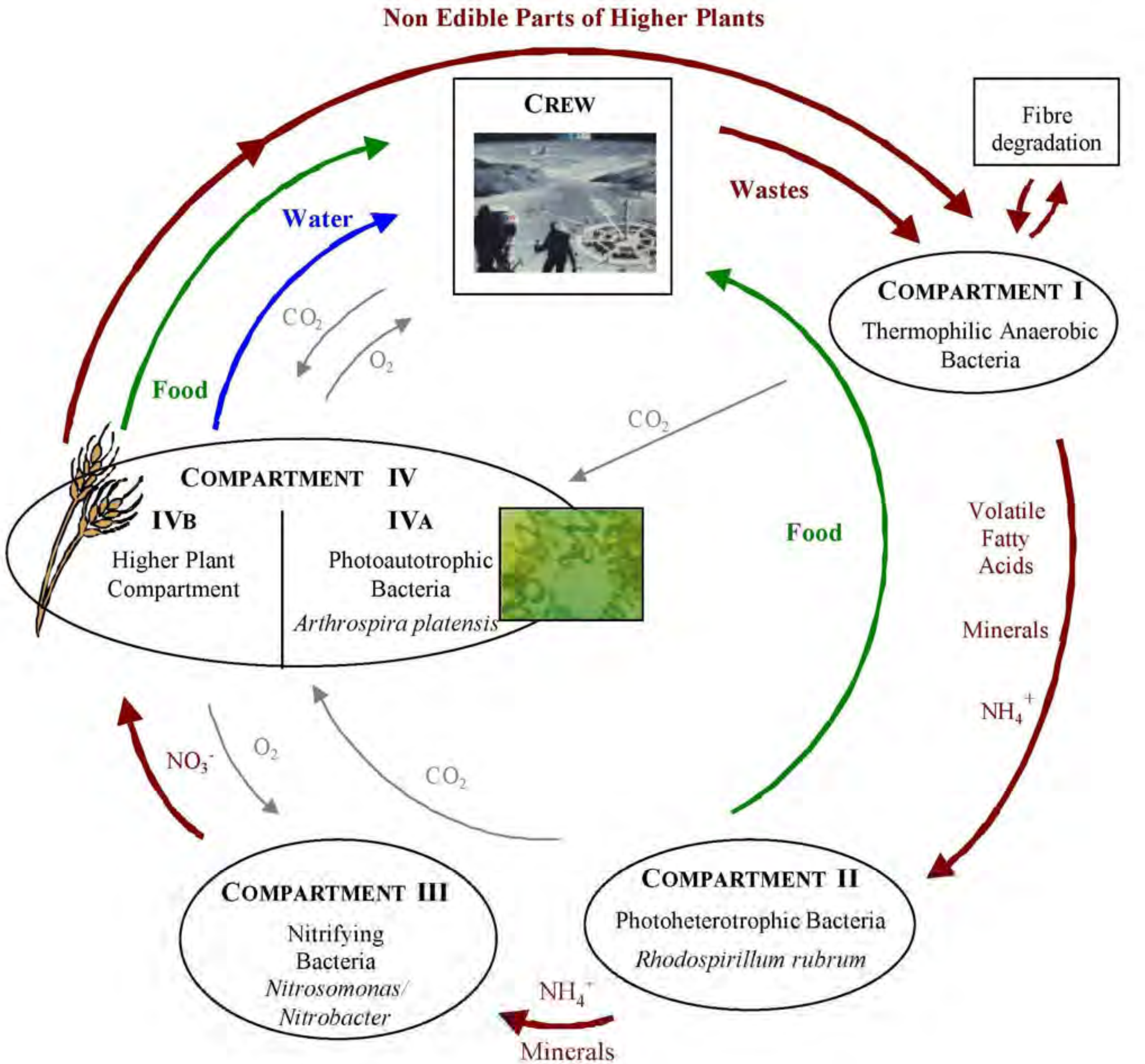
# Mass Balance at the Cellular Level



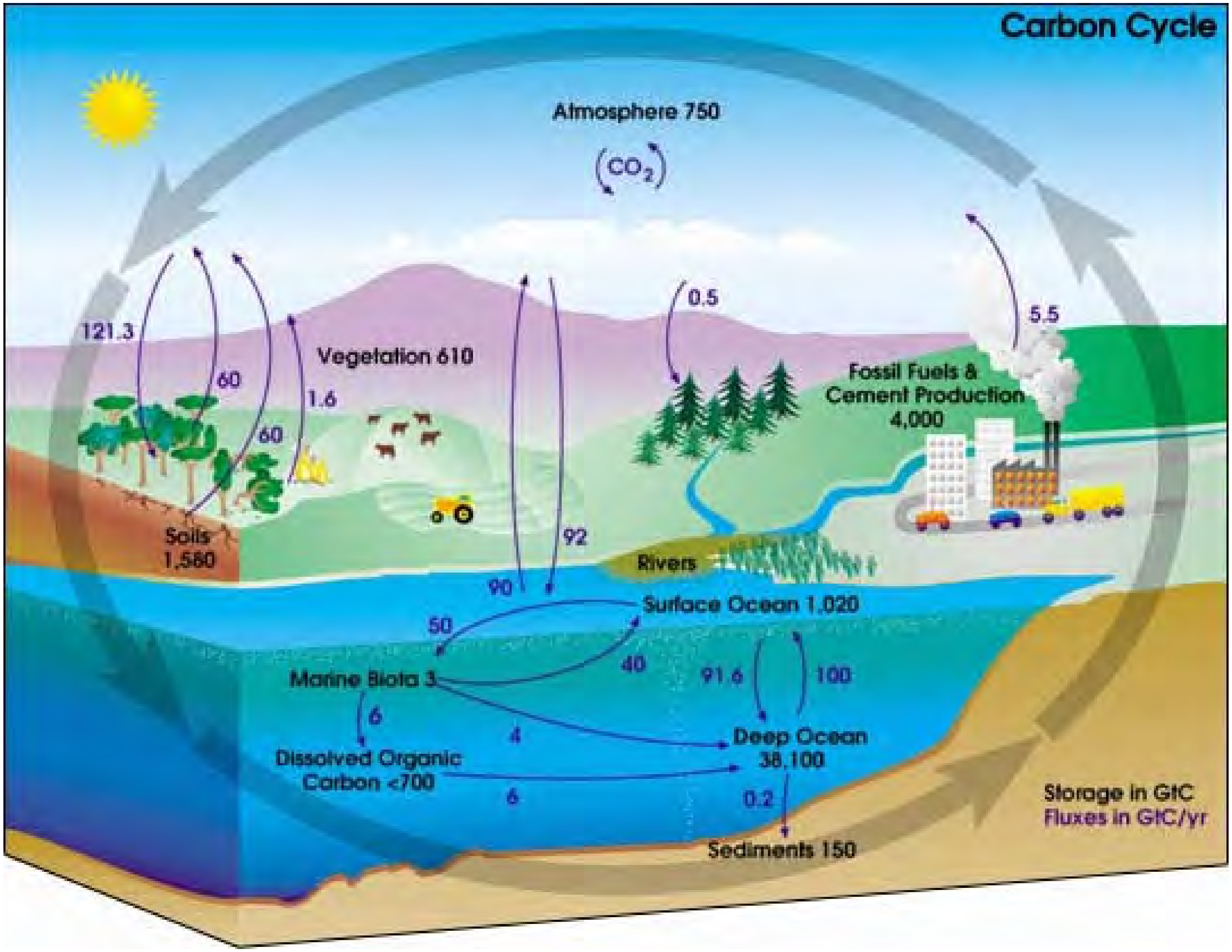
# Photosynthesis Cycle



# Mass & Energy Balances for Space Travel



# The Earth's Carbon Cycle



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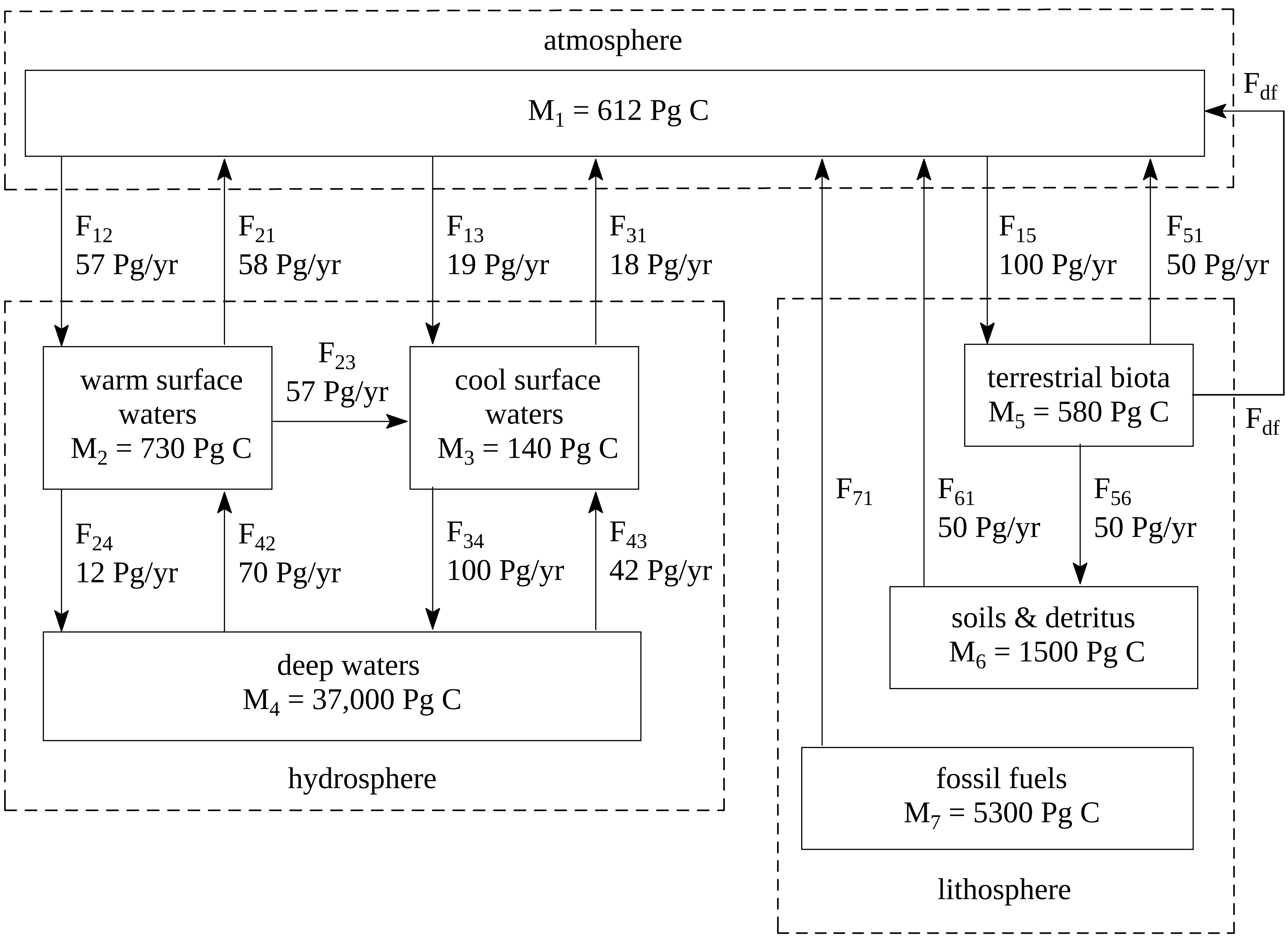


# The Earth's Carbon Cycle - Coupled Differential Equations

$$\frac{dM_1}{dt} = -(k_{12}+k_{13})M_1 - k_{15}\alpha_{\text{tb}}\frac{M_1 - M_{1,\text{threshold}}}{M_1 + M_{1,\text{saturation}}} + k_{21}\left(\frac{M_2}{730}\right)^{\beta} + k_{31}\left(\frac{M_3}{140}\right)^{\gamma}$$
$$+ k_{51}M_5 + k_{61}M_6 + F_{71} + F_{\text{df}}$$

$$\frac{dM_2}{dt} = k_{12}M_1 - (k_{23}+k_{24})M_2 - k_{21}\left(\frac{M_2}{730}\right)^{\beta} + k_{42}M_4$$

$$\frac{dM_3}{dt} = k_{13}M_1 + k_{23}M_2 - k_{34}M_3 - k_{31}\left(\frac{M_3}{140}\right)^{\gamma} + k_{43}M_4$$

$$\frac{dM_4}{dt} = k_{24}M_2 + k_{34}M_3 - (k_{42}+k_{43})M_4$$

$$\frac{dM_5}{dt} = k_{15}\alpha_{\text{tb}}\frac{M_1 - M_{\text{threshold}}}{M_1 + M_{\text{saturation}}} - (k_{51}+k_{56})M_5 - F_{\text{df}}$$

$$\frac{dM_6}{dt} = k_{56}M_5 - k_{61}M_6$$

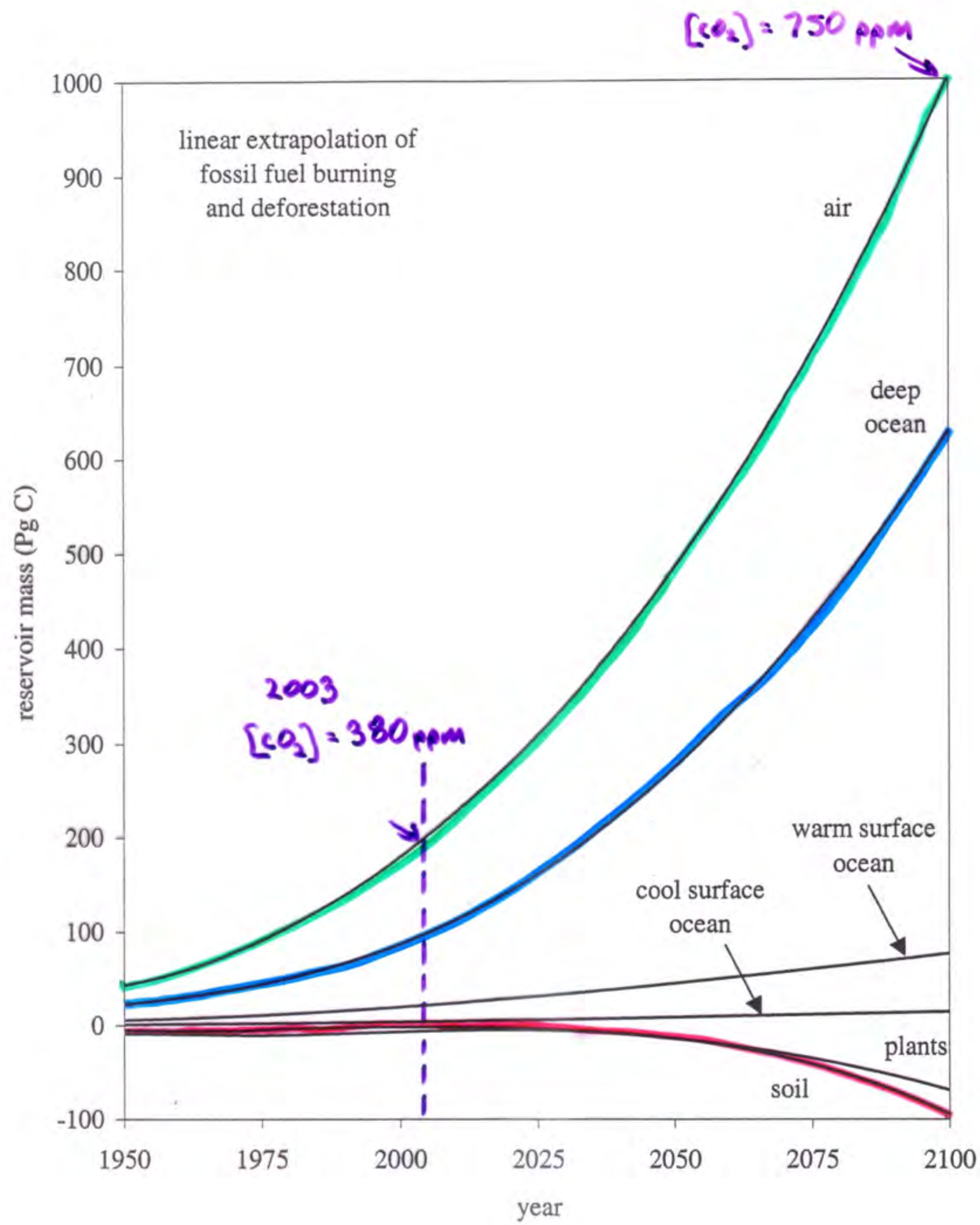
$$\frac{dM_7}{dt} = -F_{71}$$

$$\frac{d\alpha_{\text{tb}}}{dt} = \frac{-\varepsilon_{\text{df}}F_{\text{df}}}{M_{5,\text{reference}}}$$

# The Earth's Carbon Cycle - Numerical Integration

| year | F71 | Fdf | alphatb | M1 | M2 | M3 | M4 | M5 | M6 | M7 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1850.0 | 0.000 | 0.300 | 1.000 | 612.0 | 730.0 | 140.0 | 37000 | 580.0 | 1500.0 | 5300.0 |
| 1850.3 | 0.000 | 0.302 | 1.000 | 611.7 | 730.3 | 140.1 | 37000 | 579.9 | 1500.0 | 5300.0 |
| 1850.7 | 0.000 | 0.304 | 1.000 | 611.6 | 730.5 | 140.2 | 37000 | 579.7 | 1500.1 | 5300.0 |
| 1851.0 | 0.000 | 0.306 | 1.000 | 611.5 | 730.7 | 140.2 | 37000 | 579.6 | 1500.1 | 5300.0 |
| 1851.3 | 0.000 | 0.308 | 1.000 | 611.5 | 730.8 | 140.2 | 37000 | 579.5 | 1500.1 | 5300.0 |
| 1851.7 | 0.001 | 0.310 | 1.000 | 611.6 | 730.9 | 140.2 | 37000 | 579.4 | 1500.1 | 5300.0 |
| 1852.0 | 0.001 | 0.312 | 1.000 | 611.6 | 730.9 | 140.2 | 37000 | 579.3 | 1500.1 | 5300.0 |
| 1852.3 | 0.001 | 0.314 | 1.000 | 611.6 | 731.0 | 140.2 | 37000 | 579.2 | 1500.2 | 5300.0 |
| 1852.7 | 0.002 | 0.317 | 1.000 | 611.7 | 731.0 | 140.2 | 37000 | 579.1 | 1500.2 | 5300.0 |
| 1853.0 | 0.002 | 0.319 | 1.000 | 611.8 | 731.0 | 140.2 | 37000 | 579.0 | 1500.2 | 5300.0 |
| 1853.3 | 0.002 | 0.321 | 1.000 | 611.8 | 731.0 | 140.2 | 37000 | 578.9 | 1500.2 | 5300.0 |
| 1853.7 | 0.003 | 0.323 | 1.000 | 611.9 | 731.0 | 140.2 | 37000 | 578.8 | 1500.2 | 5300.0 |
| 1854.0 | 0.004 | 0.325 | 1.000 | 612.0 | 731.1 | 140.2 | 37000 | 578.7 | 1500.2 | 5300.0 |
| 1854.3 | 0.004 | 0.327 | 0.999 | 612.1 | 731.1 | 140.2 | 37000 | 578.6 | 1500.2 | 5300.0 |
| 1854.7 | 0.005 | 0.329 | 0.999 | 612.1 | 731.1 | 140.2 | 37000 | 578.6 | 1500.2 | 5300.0 |
| 1855.0 | 0.005 | 0.331 | 0.999 | 612.2 | 731.1 | 140.2 | 37000 | 578.5 | 1500.2 | 5300.0 |
| 1855.3 | 0.006 | 0.333 | 0.999 | 612.3 | 731.1 | 140.2 | 37000 | 578.4 | 1500.1 | 5300.0 |
| 1855.7 | 0.007 | 0.335 | 0.999 | 612.3 | 731.1 | 140.2 | 37000 | 578.4 | 1500.1 | 5300.0 |
| 1856.0 | 0.008 | 0.337 | 0.999 | 612.4 | 731.1 | 140.2 | 37000 | 578.3 | 1500.1 | 5300.0 |
| 1856.3 | 0.009 | 0.339 | 0.999 | 612.5 | 731.1 | 140.2 | 37000 | 578.2 | 1500.1 | 5300.0 |
| 1856.7 | 0.010 | 0.341 | 0.999 | 612.5 | 731.1 | 140.2 | 37000 | 578.2 | 1500.1 | 5300.0 |

# The Earth’s Carbon Cycle - Numerical Integration



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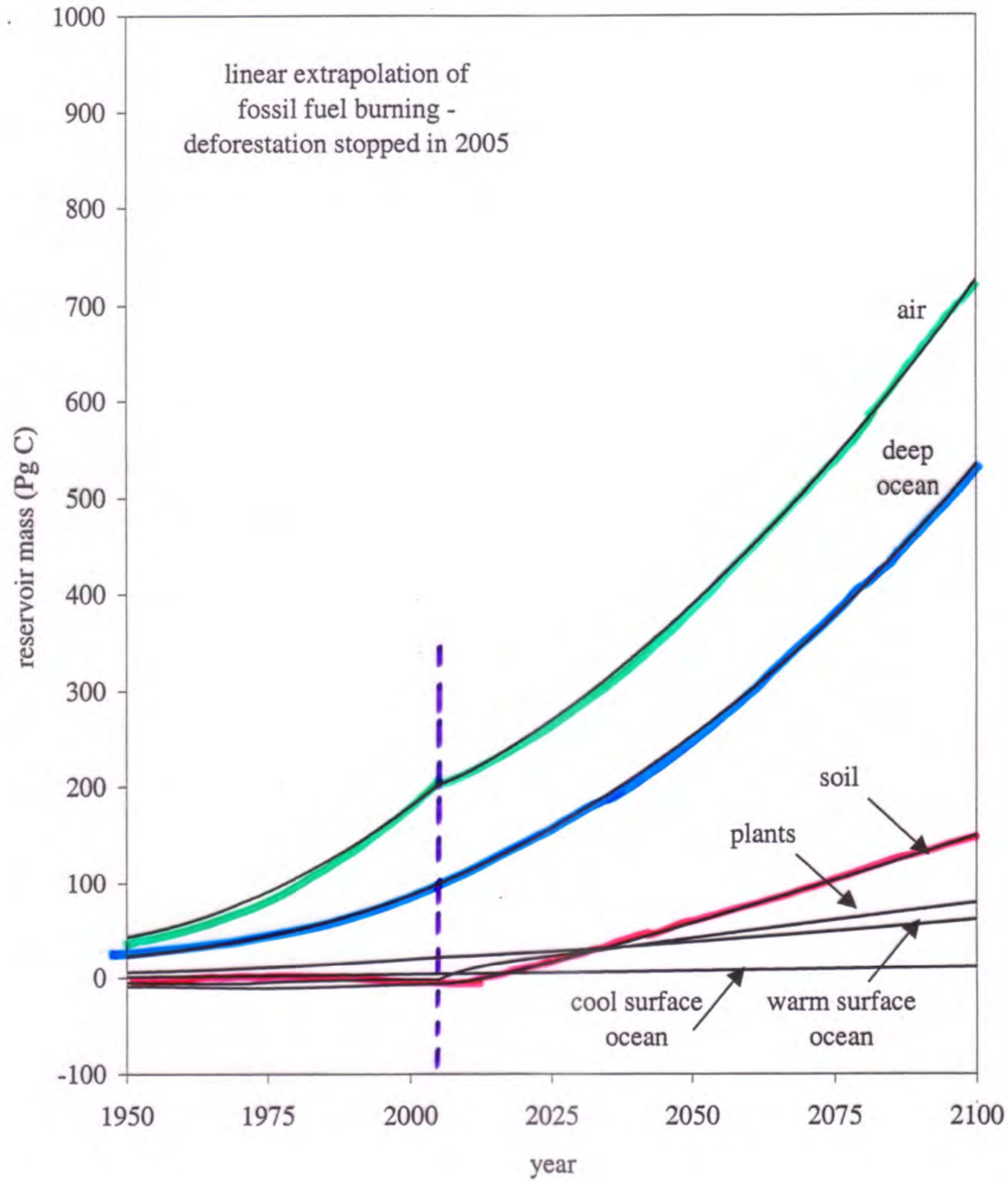

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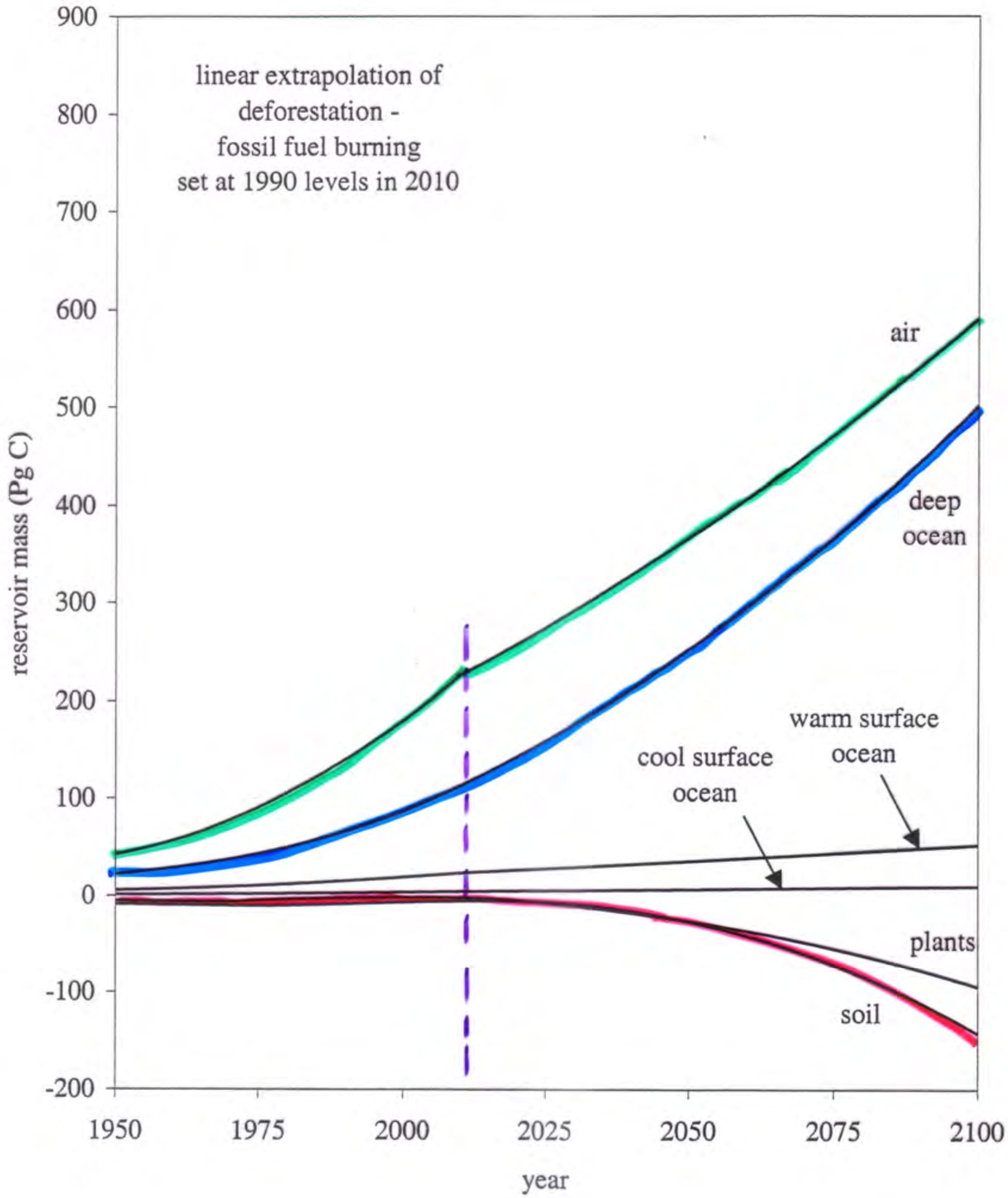

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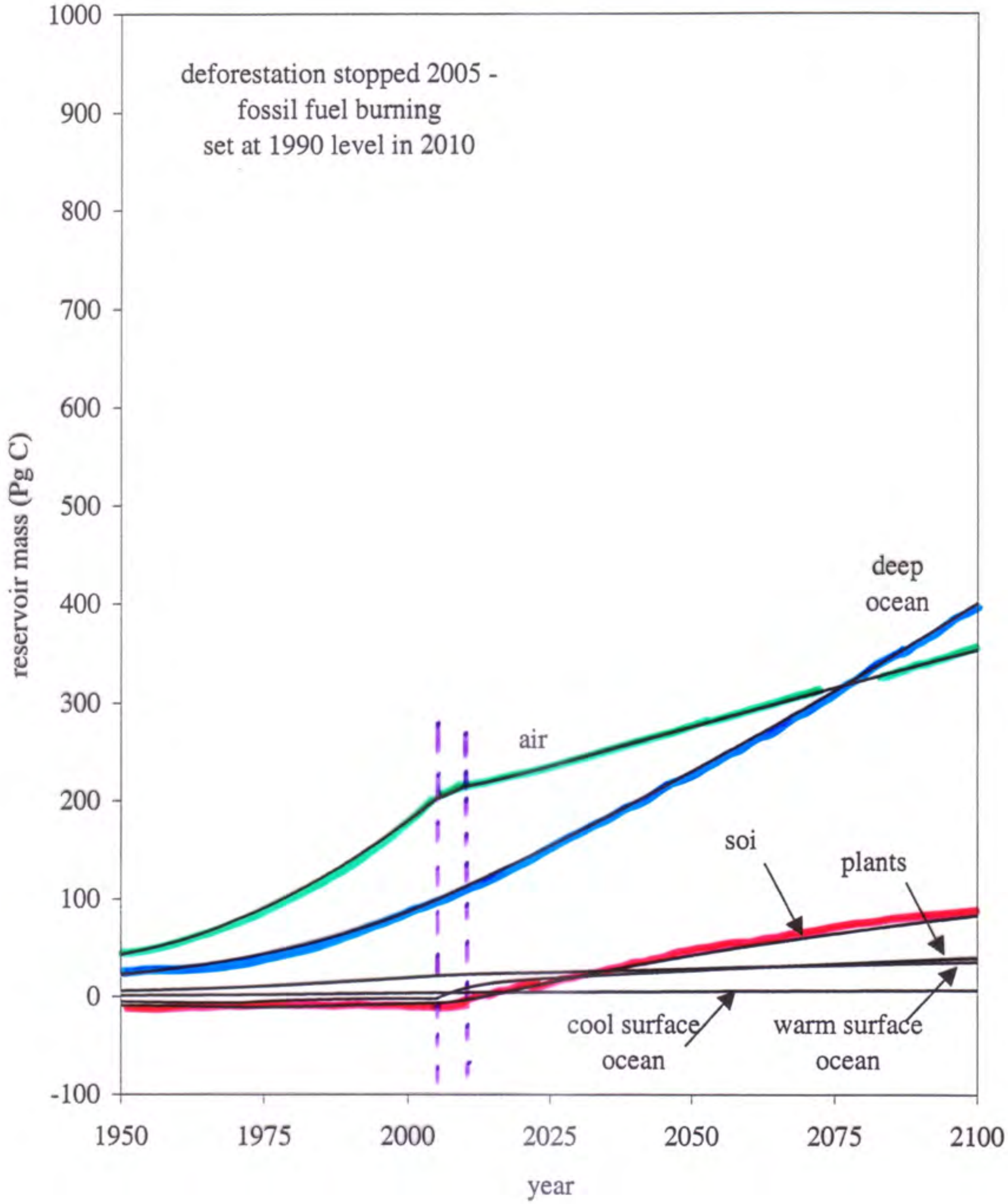


# Mathematical Mass & Energy Balances

- Define nomenclature.
- Show system borders and state assumptions.
- State source of equation -

  "apply conservation of mass" or

  "reaction specification" or

  "stream composition."
- Describe derivation.

  "Substitute eqns (1) and (2) into eqn (3)."
- Box answer:

  number with no insignificant figures

  and units, such as kJ/min.

# Energy Balances

1. Cannot calculate energy of a mass stream;

    **cannot** state $q_1 = 100$ kJ/min

   Must calculate the change in energy of a mass stream;

    must calculate $\Delta q_{1 \rightarrow 2} = q_2 - q_1$

2. Cannot measure $\Delta q$; must measure $\Delta T$ *or* $\Delta$*phase*

   and use thermodynamics to convert to energy.

3. Simple mass units can be complex energy units.

   Create an equivalent unit of elementary energy units.

An elementary energy unit has -

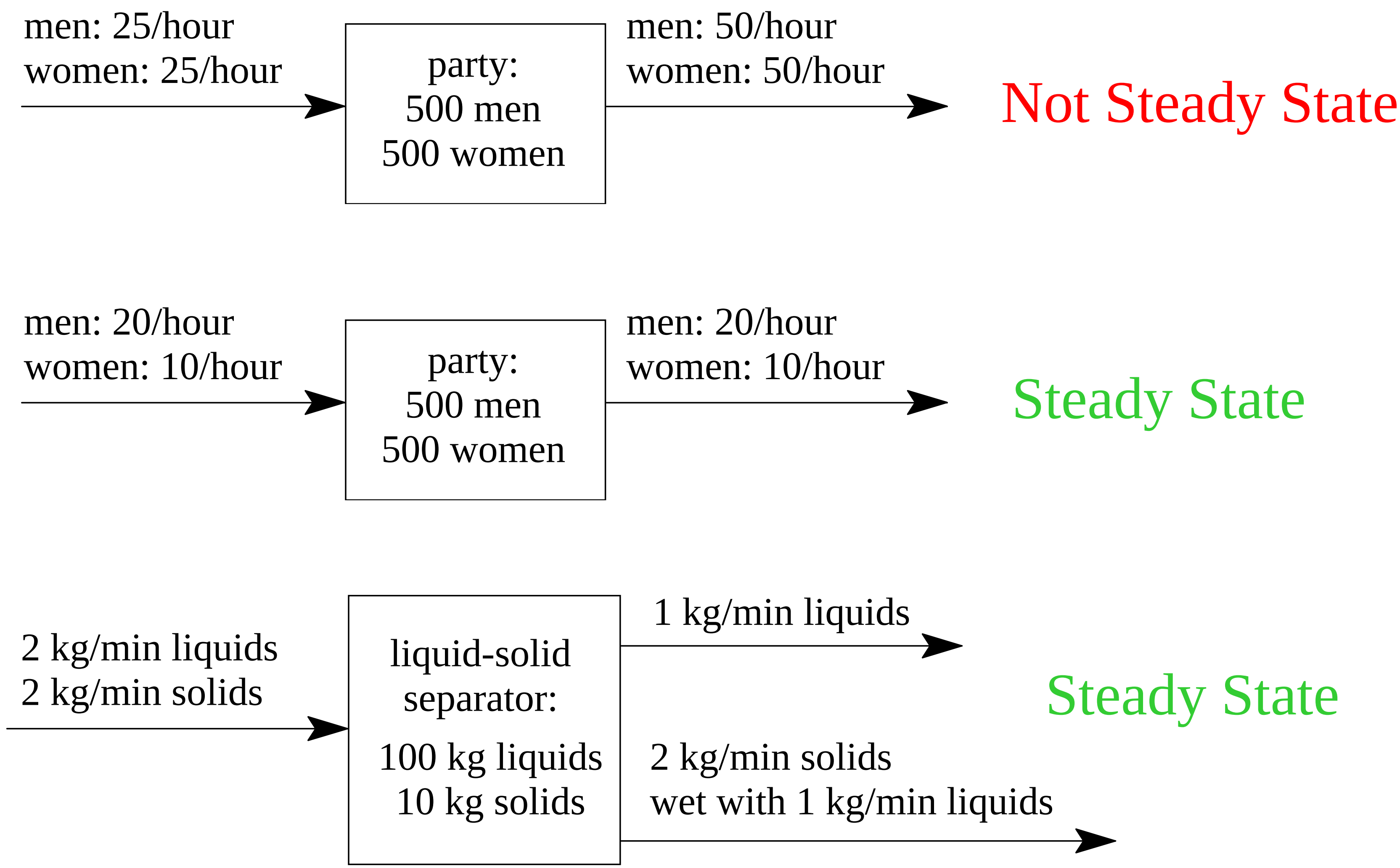
one mass stream in, one mass stream out,

one energy change; $\Delta T$ *or* $\Delta$*phase*, and

***all*** mass passing through the unit is heated or changes phase.

# Mathematical Modeling

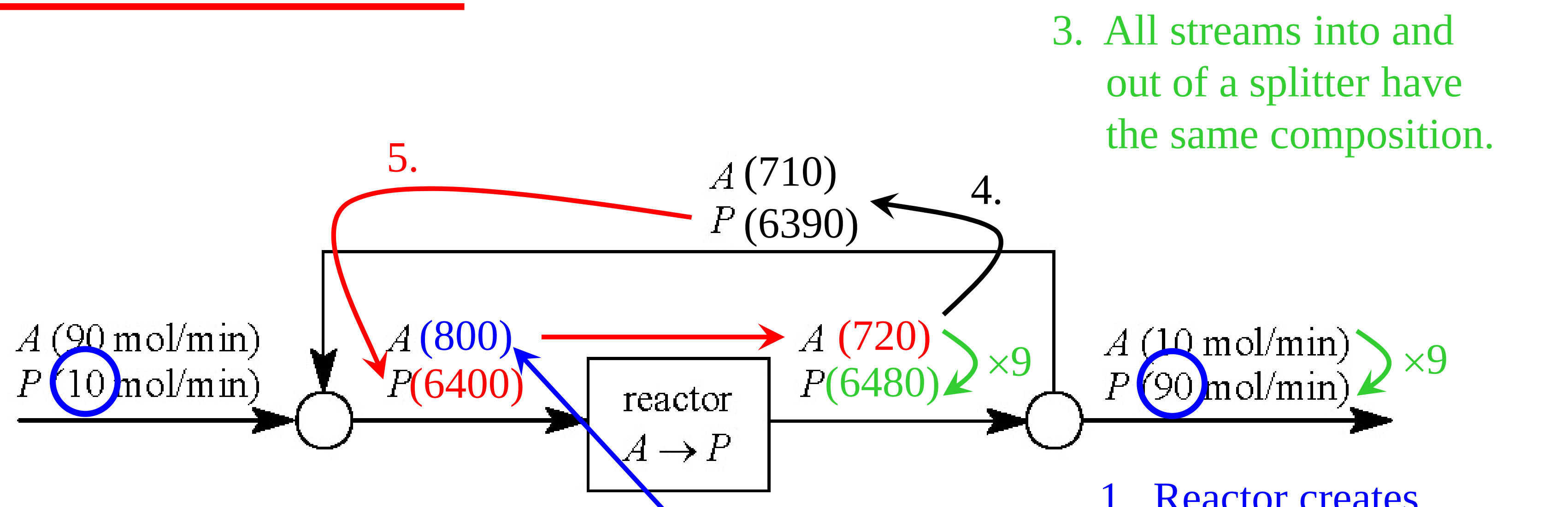
## Are These Flow Rates Consistent with Steady State?



# Mathematical Modeling - Informal Mass Balances

**3.48** *A* and *P* cannot be separated. The process below increases the ratio of *P* to *A* by the reaction $A \to P$. The reactor converts 10% of the *A* that enters.

2.

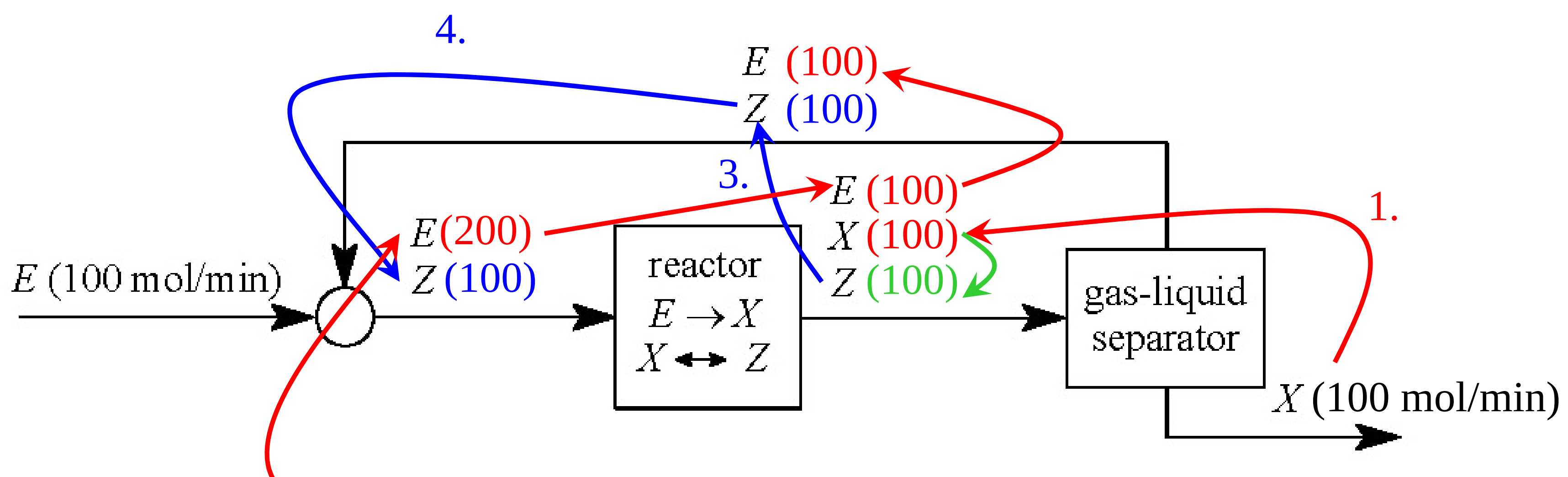



Calculate the flow rates of *A* and *P* in all streams.

$$\frac{80}{0.1} = 800$$

# Mathematical Modeling - Informal Mass Balances

**3.50** The process below produces $X$ by the reaction $E \rightarrow X$. The reactor converts 50% of the $E$ that enters. 5.
Product $X$ is in equilibrium with useless by-product $Z$. The ratio of $X$ to $Z$ is 1:1. 2.



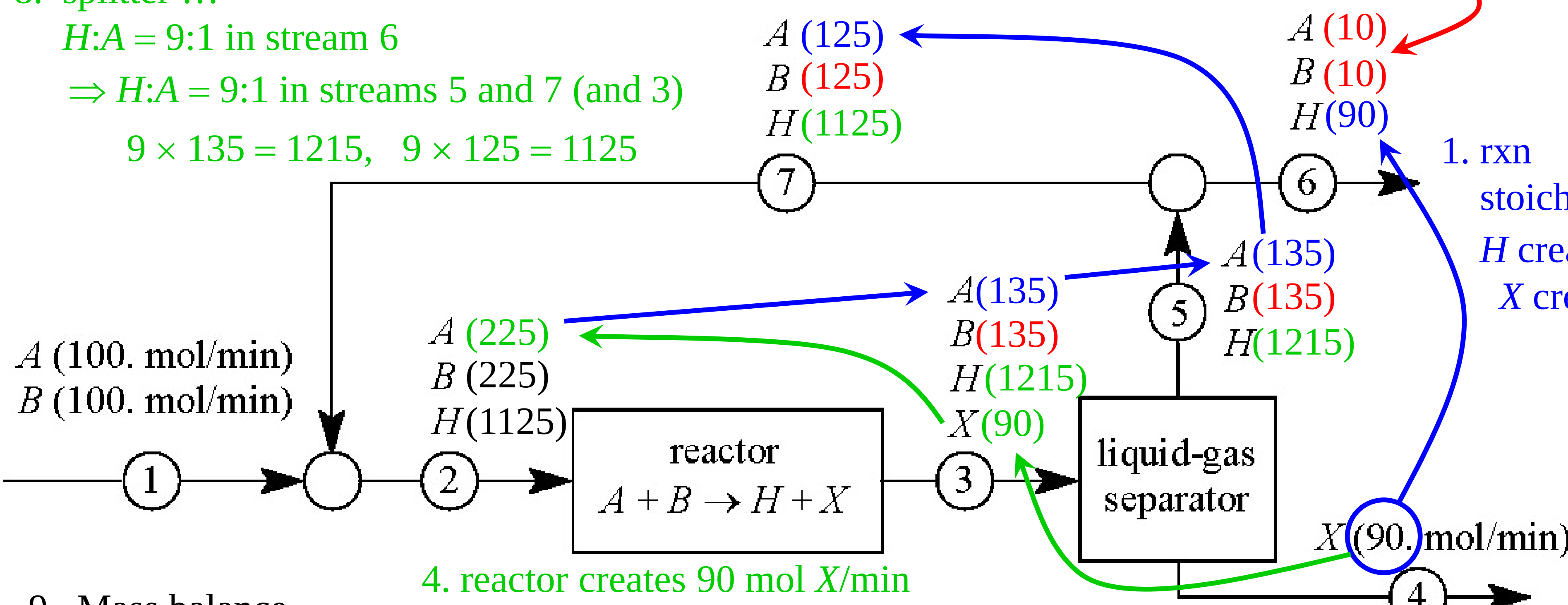

Calculate the flow rates of $E$, $X$, and $Z$ in all streams.

$$E: \frac{100}{0.5} = 200$$

5. Reactor creates 100 mol $X$/min. *and* 0 mol $Z$/min.

# Informal Mass Balance – Exercise 3.51

**3.51** The process below produces $X$ using the reaction $A + B \rightarrow H + X$. The reactor conversion is 40.%; if 10 mol $A$ and 10 mol $B$ enter the reactor, 6 mol $A$ and 6 mol $B$ leave the reactor.




1. rxn stoichiometry: $H$ created = $X$ created

2. mols conserved in rxn: 200 mols in → 200 mols out
$\Rightarrow (A + B)_{out} = 200 - 90 - 90 = 20$
rxn stoichiometry: $A = B$
$\Rightarrow \quad A = B = 10$

3. mass balance on separator

4. reactor creates 90 mol $X$/min
reactor conversion = 40%
$\Rightarrow$ $A$ into reactor = 90/0.40 = 225

5. reactor consumes 90 mol $A$/min
$\Rightarrow$ $A$ out of reactor = 225 – 90 = 135

6. mass balance on splitter: 135 – 10 = 125

7. All streams entering and leaving a splitter are the same composition.
$A$:$B$ = 1:1 in stream 6
$\Rightarrow$ $A$:$B$ = 1:1 in streams 5 and 7 (and 3)

8. splitter …
$H$:$A$ = 9:1 in stream 6
$\Rightarrow$ $H$:$A$ = 9:1 in streams 5 and 7 (and 3)
$9 \times 135 = 1215, \quad 9 \times 125 = 1125$

9. Mass balance on combiner

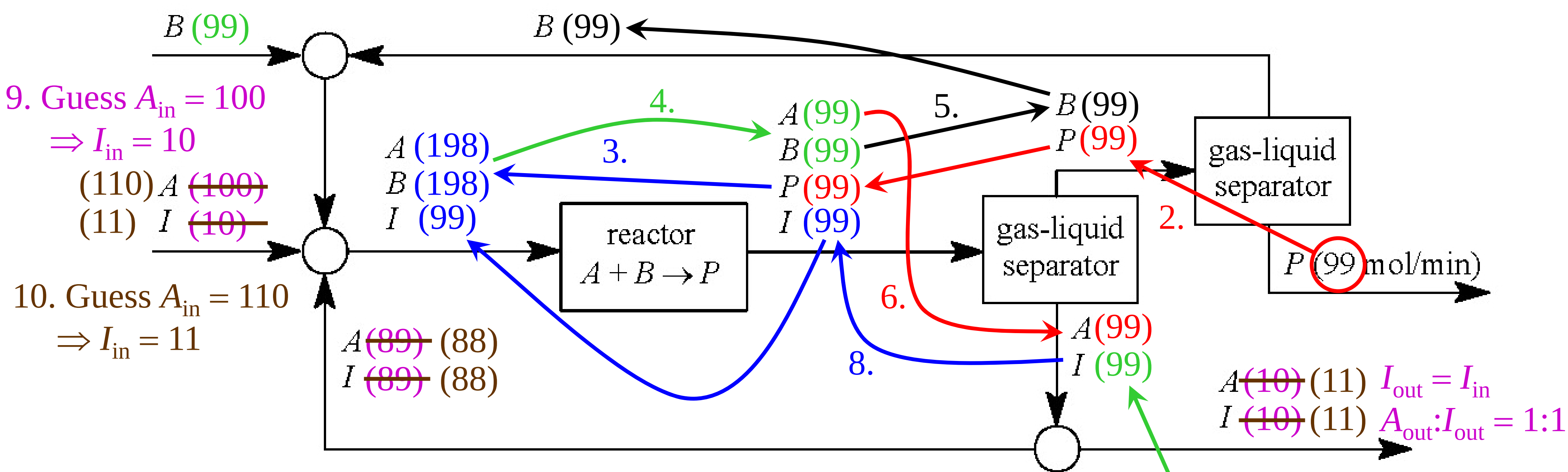
# Mathematical Modeling - Informal Mass Balances

3. 9.

**3.52** The reactor below converts 50% of $A$ and $B$ for equal molar flow rates of $A$ and $B$. The ratio of $A$ to $I$ in the feed is 10 to 1. The ratio of $A$ to $I$ in the purge output is 1 to 1. ← 7.

1. Overall mass balance:

$B_{in} = B_{out} + P_{out}$




8a. No guess

$$\left.\begin{array}{l} A_{out} = I_{out} \\ I_{out} = I_{in} \\ A_{in} = 10 I_{in} \end{array}\right\} \quad A_{in} = 10 A_{out}$$

$$A + B \rightarrow P$$
$$P_{out} = 99$$
$$A_{in} = A_{out} + 99$$
$$10 A_{out} = A_{out} + 99$$

$$A_{out} = 11,\ A_{in} = 110$$

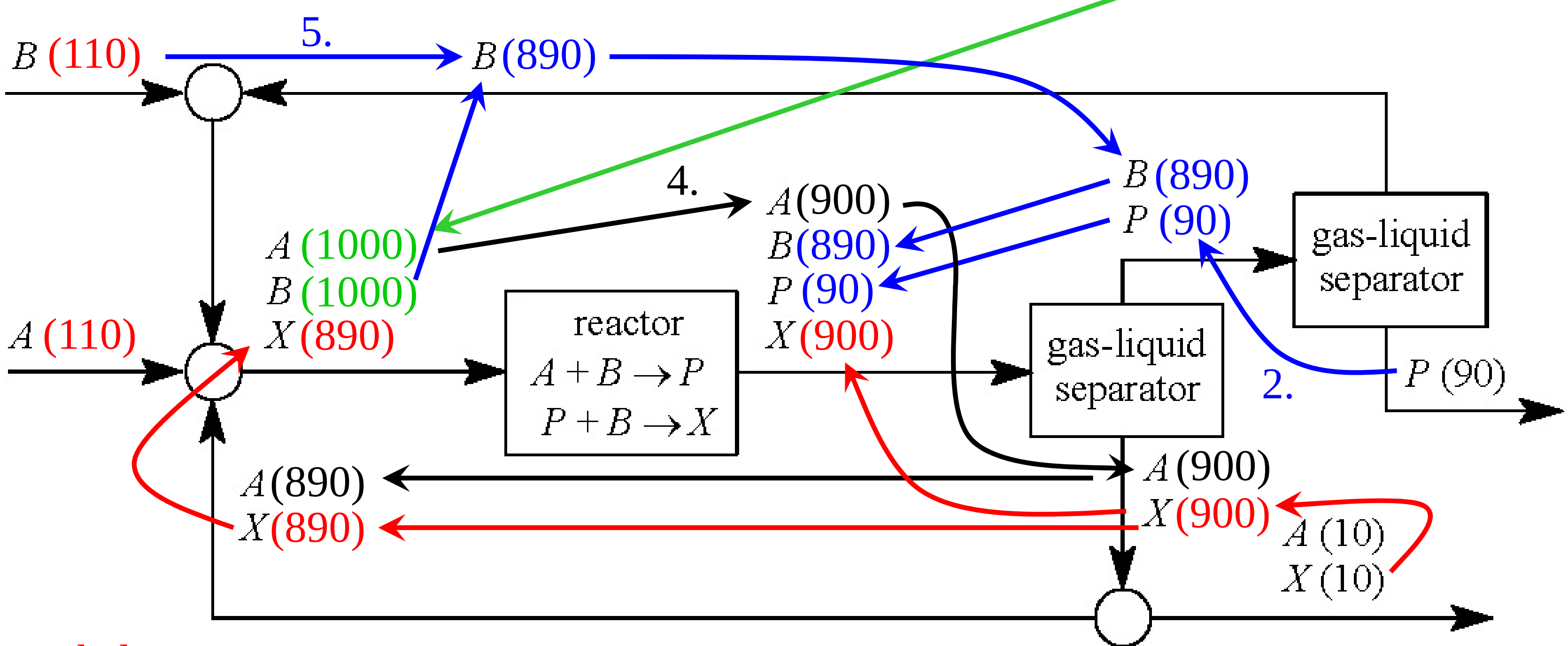
7. All streams into and out of a splitter have the same composition.

# Mathematical Modeling - Informal Mass Balances

3.

**3.56** The reactor below converts 10% of $A$ and $B$ for equal molar flow rates of $A$ and $B$. Product $P$ also reacts with $B$ to form by-product $X$. Separating $A$ from $X$ is impractical because $A$ and $X$ have the same melting point and boiling point; $X$ is removed from the process by a purge which also removes some $A$.

3. $P_{created} = P_{out} + X_{out} = 90 + 10 = 100$ $\quad$ $A$ into reactor $=$ $B$ into reactor $= \frac{100}{0.1} = 1000$




1. Overall mass balances

$A_{in} = A_{out} + P_{out} + X_{out}$

$= 10 + 90 + 10 = 110$

$B_{in} = B_{out} + P_{out} + 2X_{out}$

$= 0 + 90 + 2\times 10 = 110$

6. All streams into and out of a splitter have the same composition.

# Prelim 3 2025 Statistics

Mean: 76 / 120 (63%)
Std. Deviation: 28

A - K: Angel (Front of room)
L - Z: Lara (Back of room)

*Solution is posted.*

Problem 1: 19 ± 7 / 25 (75%)
Problem 2: 28 ± 8 / 35 (79%)
Problem 3: 30 ± 19 / 60 (50%)