NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

RE1015: Bio- and Chemical Engineering Fundamentals and Applications

Week 9

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16 Oct 2024

Outline

- Fundamentals
- Batch versus continuous systems (Group Discussion)
- Transient versus steady state processes
- General equation for material balance
- Material balance for continuous systems operating at steady state
- Representing chemical processes using a block diagram
- Points to note when performing a material balance

- Problem 1: Block diagram
- Problem 2: Humidifier
- Problem 3: Green ammonia synthesis
- Pop quiz **(1715 h)**

Course Schedule

Week	Lecture	Tutorial	Additional Details
08	The Role of Chemical Engineers in Implementing Singapore's Decarbonization Strategy **(09 Oct 2024)**	Decarbonization strategies, pop-quiz.	Pathways to decarbonization, using CO_2 as a raw material for manufacturing chemicals and construction materials, the hydrogen economy, upcycling plastic/food waste into value.
09	Mass and Energy Balances: The *sine qua non* of Chemical Engineering (**16 Oct 2024)**	Problem solving: ammonia synthesis from air, pop-quiz.	Conservation of mass, conservation of energy, mass and energy balance using recycle streams.
10	The Second Law of Thermodynamics: All Energy Cannot Become Useful Work **(18 Oct 2024)**	Problem solving: Understanding how Internal Combustion Engines work, pop-quiz.	Phenomenological origins of the second law of thermodynamics, applications of the second law of thermodynamics to different power units like the internal combustion engine, hybrid engine, and fuel cell vehicles.

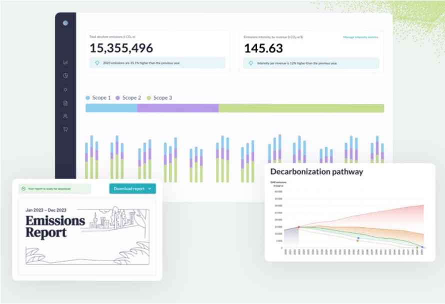
Course Schedule

11	Chemical Kinetics and Chemical Equilibrium: Understanding the Rate of Change (**30 Oct 2024)**	Problem solving: Understanding equilibrium limitations to ammonia synthesis, reactor design, pop-quiz.	The law of mass action, chemical equilibrium, Le Chatelier's principle, chemical reactions in series and in parallel. The overall theme will be ammonia synthesis and methanol synthesis from CO_2.
12	Catalysts: The Philosopher's Stones that Enable Chemical Transformations **(06 Nov. 2024)**	Guest lecture: Dr. Saifudin Abubakar, Corporate Lab Director, ExxonMobil **(To be confirmed)**	The Sabatier principle, role of quantum chemistry in accelerating the design of catalysts, descriptors of catalytic reactivity and selectivity, applications of catalyst design principles to fuel cells.
13	How Chemical Engineers will Harness Artificial Intelligence to Address Grand Challenges in Sustainability. **(13 Nov. 2024)**	Group Discussion: Decarbonization strategies, pop-quiz.	Selected examples of Artificial Intelligence based methods, data mining, and accelerated materials discovery that will enable chemical engineers to solve grand challenges in sustainability.

Start-ups in Decarbonisation in Singapore

Unravel Carbon

Help companies to measure, report, and reduce their carbon emissions



https://www.unravelcarbon.com

Xinterra

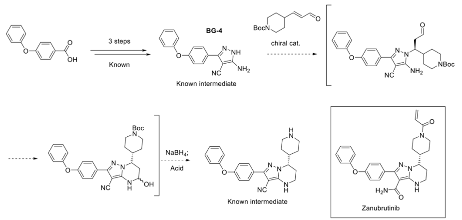
Accelerated development of materials using AI technology

High-throughput experimental platform to design extile that captures CO_2 from air. CO_2 is removed as carbonates when clothes are washed. 20 T-shirts remove as much CO_2 as a mature tree does in a day.

Accelerated Materials

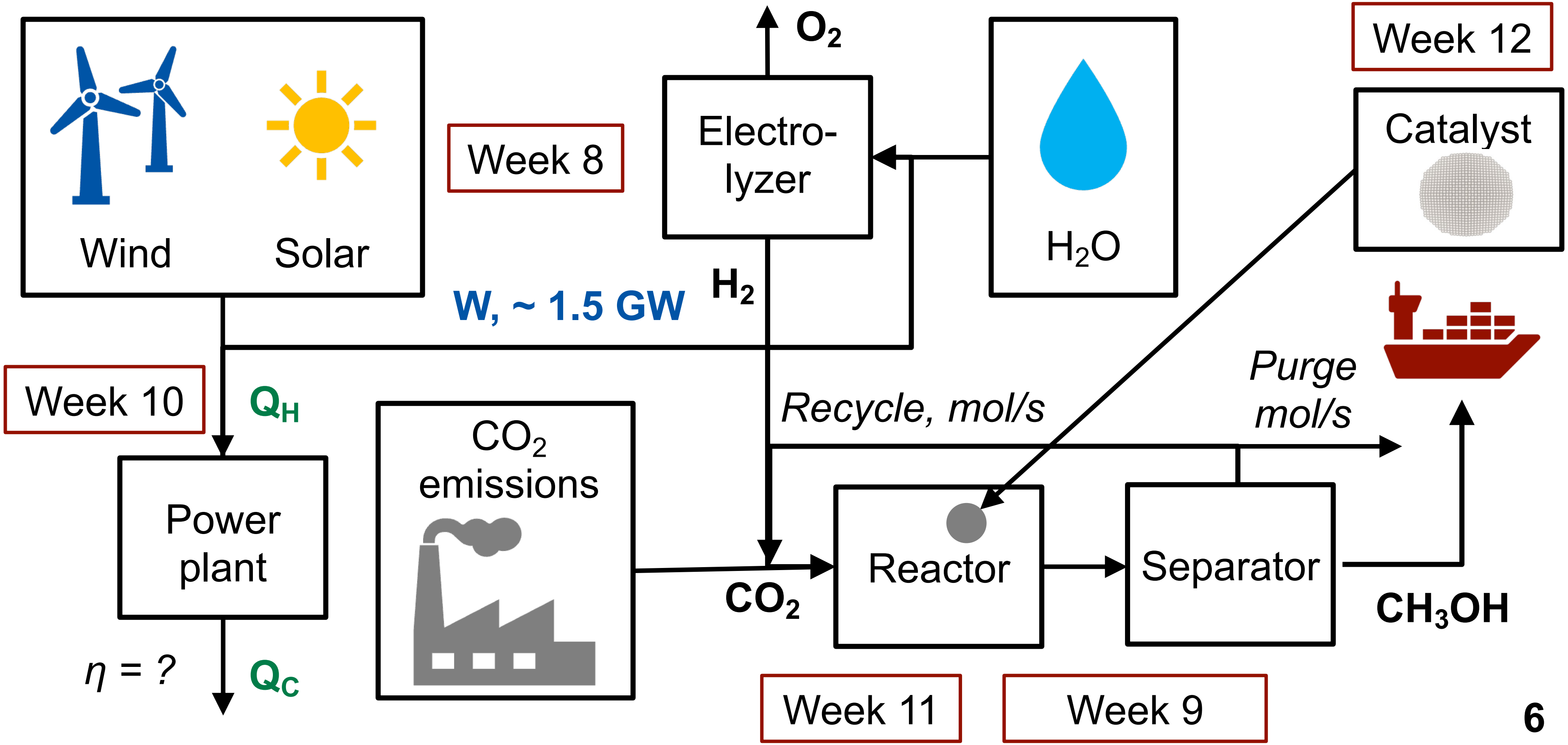
Scaling up the synthesis of nanomaterials and pharmaceuticals like anti-cancer drug intermediates.

Suite of machine learning tools to accelerate the scale-up process



Scheme 1. Schematic of Zanubrutinib synthesis pathway, showing key intermediates, including BG-4.

1 Million Tons per Annum of Green Methanol for 25 Container Ships



Molecular weight of compounds (use mass numbers from periodic table)

CH_3OH: 12 + 3+ 16 + 1 = 34 g mol^{-1}

Calculate number of moles

How many moles of H_2O are present in 1 bathtub having a volume of 160 litres?

Volume = 160 litres = 0.160 m^3. Density of water = 1000 kg m^{-3}.
Mass = 0.160x1000 = 160 kg
Molecular weight of H_2O: 2 + 16 = 18 g mol^{-1}
Moles of water = $160\ \cancel{kg} \times 1000\ \frac{\cancel{g}}{\cancel{kg}} \times \frac{1}{18}\ \frac{mol}{\cancel{g}}$ = **8888.89 moles**

Balance chemical reactions

$2\,CO_2 + 6\,H_2 \leftrightarrow C_2H_5OH + 3\,H_2O$

Unit conversions *(patient you must be...)*

The flow rate of high pressure hydrogen gas is 100 mol h^{-1}. Convert the flow rate into m^3 s^{-1}. Assume compressed hydrogen has a density of 20 kg m^{-3}.

$$100\ \frac{mol}{h}\times\frac{2}{1}\frac{g}{mol}$$

$$100\ \frac{mol}{h}\times\frac{2}{1}\frac{g}{mol}\times\frac{1}{1000}\frac{kg}{g}$$

$$100\ \frac{mol}{h}\times\frac{2}{1}\frac{g}{mol}\times\frac{1}{1000}\frac{kg}{g}\times\frac{1}{20}\frac{m^3}{kg}$$

$$100\ \frac{mol}{h}\times\frac{2}{1}\frac{g}{mol}\times\frac{1}{1000}\frac{kg}{g}\times\frac{1}{20}\frac{m^3}{kg}\times\frac{1}{3600}\frac{h}{s}\ = 2.78\times10^{-6}\frac{m^3}{s}$$

Let us practice some unit conversions with Rebel General Han Solo

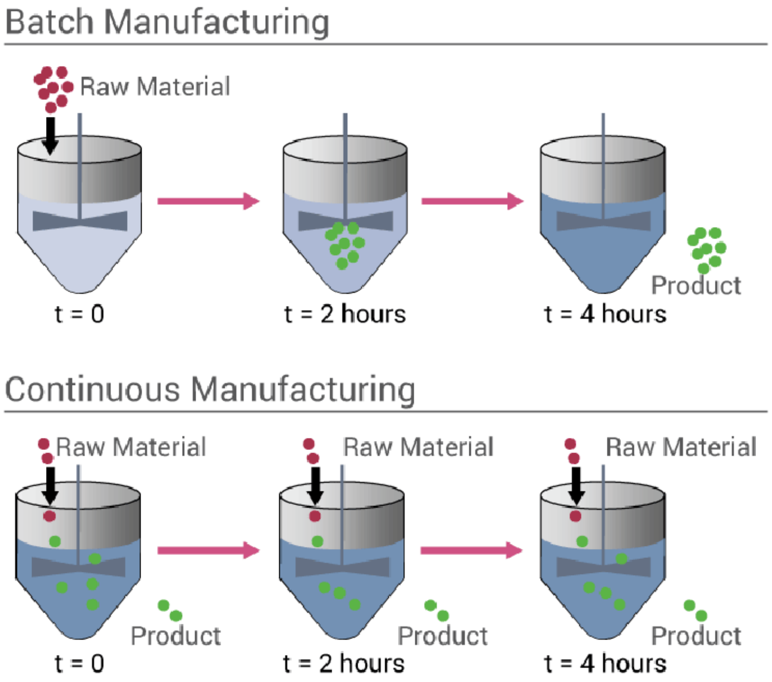
Han Solo claims in the Star Wars series that his beloved Millennium Falcon did the kesselrun in 12 parsecs.

Assume the millenium falcon goes 1000x the speed of light on its hyperdrive.

What was the distance of the kesselrun in light years?
How long did Solo's journey take in days?

Useful information: 1 parsec is the distance at which 1 astronomical unit subtends an angle of 1 arc second.
Speed of light 299 792 458 m/s

Batch versus Continuous Systems



A simple depiction of two types of manufacturing. Batch manufacturing: the material(s) is charged before the start of processing and the product is discharged at the end of processing. Continuous manufacturing: material(s) and the product are simultaneously charged and discharged from the process, respectively

Batch: Process parameters (e.g. T, conc.) vary as a function of time (commonly used in pharmaceutical and food industries)

Continuous: Process parameters do not vary as a function of time once <u>steady-state</u> is reached (standard practice in oil refinery, petrochemicals)

Batch versus Continuous Systems (Group Discussion)

Which situations demand batch processes? Which situations need continuous processes? Discuss the advantages of batch versus continuous processes using the following points. Discuss within your groups first (five minutes), then we discuss together (five minutes).

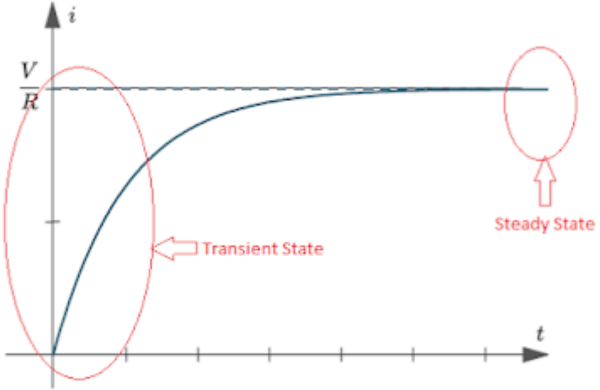
(1). Scale of manufacture small scale, batch, large scale continuous

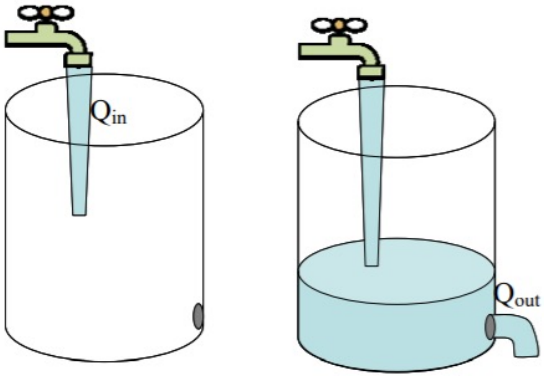
(2). Availability of utilities, raw material, labour costs if expensive, continuous

(3). Quality control of product batch have better quality control

(4). Demand for product. Continuous mode if the demand is high.

Transient versus Steady State Processes



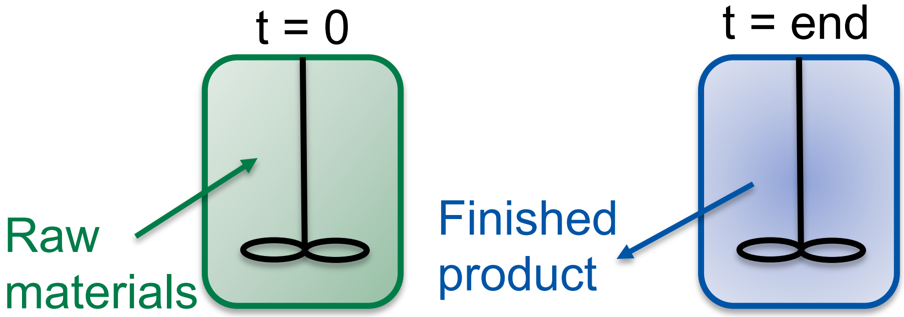


Transient State (e.g., semi-batch system):
- Net gain/loss of mass in the system
- Amount of mass changes as a function of time

Steady State (continuous system):
- No net gain/loss of mass in the system after a "start-up" period
- Constant amount of mass in the system as a function of time

General Equation for Material Balance

Batch systems



Accumulation = Generation - Consumption

Generation and consumption can occur due to chemical reactions.

Continuous systems

Accumulation = Mass flow in – Mass flow out + Generation - Consumption

Continuous processes have streams flowing materials into, and out of the system.

Material Balance Equation for Continuous Processes at Steady State

Continuous systems

Accumulation = 0 = Mass flow in – Mass flow out + Generation - Consumption

At steady state, no accumulation of mass within the system.

EXAMPLE 4.2-1 ***The General Balance Equation***

Each year 50,000 people move into a city, 75,000 people move out, 22,000 are born, and 19,000 die. Write a balance on the population of the city.

SOLUTION Let P denote people:

$$\text{input} + \text{generation} - \text{output} - \text{consumption} = \text{accumulation}$$

$$50{,}000 \frac{P}{\text{yr}} + 22{,}000 \frac{P}{\text{yr}} - 75{,}000 \frac{P}{\text{yr}} - 19{,}000 \frac{P}{\text{yr}} = A\left(\frac{P}{\text{yr}}\right)$$

$$\Downarrow$$

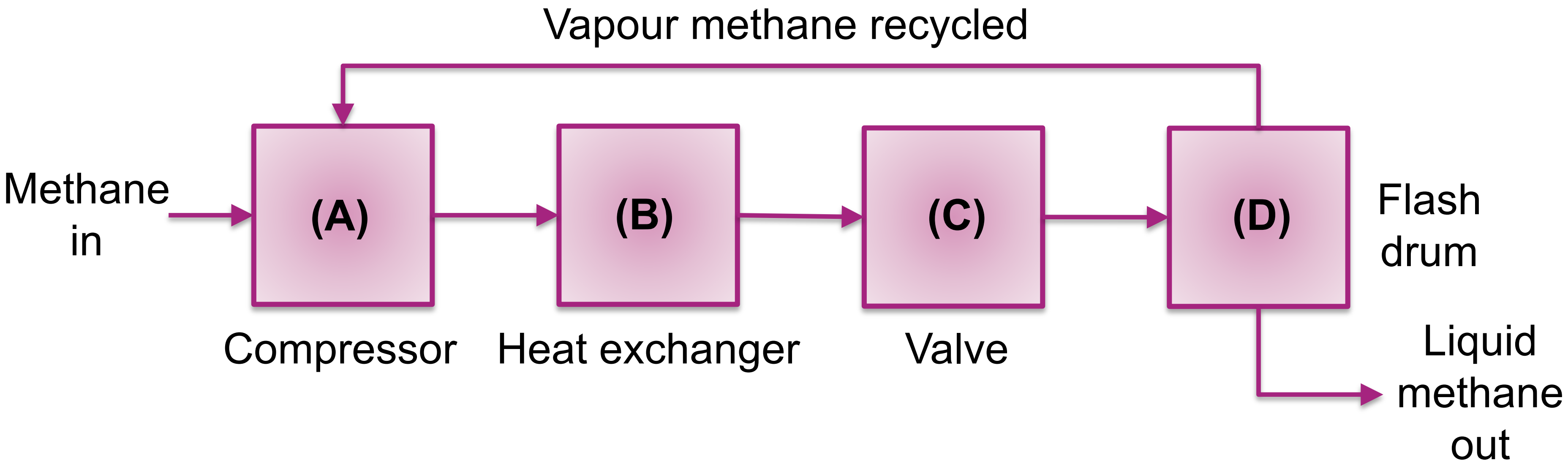
$$A = -22{,}000 \frac{P}{\text{yr}}$$

Each year the city's population decreases by 22,000 people.

Representing Chemical Processes using Block Diagrams

Methane is compressed to liquified natural gas for transoceanic shipment. Singapore is one of the world's largest hubs for methane liquefaction. Methane is first compressed to a high pressure and temperature using a compressor (A). The hot gas is then cooled in a heat exchanger (B). The high pressure cooled gas is then expanded over a valve (C) to atmospheric pressure. A fraction of the methane vapours condense forming liquified natural gas, while the rest remains in the gas phase. The liquid and vapour streams are separated in a flash drum (D). The vapour stream is recycled back to the compressor. Represent the process using a block diagram

Representing Chemical Processes using Block Diagrams



Points to Note When Performing a Material Balance

(1). Draw a block diagram for the process.

(2). Number all streams.

(3). Write down the composition and flow rates of all streams in consistent units (e.g., either mol, mol%, mol/h, or kg, kg%, kg/h). Where necessary, convert units appropriately.

(4). Write down mass balance equations over every block within the diagram. Also write down the overall mass balance for the process.

(5). Determine the known variables, and the unknown variables. Make sure that there are sufficient equations relating the unknown variables such that they can be solved.