

Balance and Process Fundamentals

Balances are simple accounting procedures used to aid in the overall analysis of a process 's viability.

Exactly *how* ; a process is run, often determines much regarding what the balance equations will look like. What are some of the characteristics that a running process may have ?

- Characterize system operation
 - # Give original examples of (and identify) batch, semi - batch, continuous, steady, and transient processes
 - # Define open system, closed system, adiabatic, isothermal

What are quantities for which we can write balances ? Just like a checkbook, we can have inputs / deposits / credits and we can have outputs / withdrawals / debits. What are some of the *ways* in which these ins and outs can occur ? What happens if we put more in than we take out ?

- Explain the origin and physical meaning of each of the terms in the General Mass Balance Equation
- Write a General Energy Balance Equation
 - # Explain the origin and physical meaning of each of the terms in the General Energy Balance Equation
 - # Explain the difference between shaft work and flow work
 - # Simplify the appropriate form of the Energy Balance Equation

Now that we have written our balance equations, how can we concisely depict the information that we require to actually *do* the balance (or show our results after we have completed the balance) ?

- Draw and label a flowchart from a process description
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Process Classification

One of the first things that ChE's need to know about processes is the many different ways in which we may operate a process.

There are three major classification of processes:

DEFINITION

*In a **batch** process, material is placed in the vessel at the start and (only) removed at the end --no material is exchanged with the surroundings during the process.*

Batch Examples: baking cookies, fermentations, small-scale chemicals (pharmaceuticals)

DEFINITION

*In a **continuous** process, material flows into and out of the process during the entire duration.*

Continuous Examples: pool filter, distillation processes

DEFINITION

*A **semi-batch** process is one that does not neatly fit into either of the other categories (i.e., it is a catch-all classification).*

Semi-Batch Examples: washing machine, fermentation with purge.

Process Operation

Each of the above classes of process may be further distinguished by their mode of operation with respect to time.

Continuous processes may be run:

DEFINITION

*At **steady-state**, none of the process variables change with time (if we ignore small, random fluctuations).*

or it may be run

DEFINITION

*At **unsteady-state**, the process variables change with time. (One class of unsteady-state processes are oscillatory, where they process variables change with time in a regular way. All other unsteady processes may be called Transient meaning that the process variables continuously evolve over time).*

OUTCOME

Give original examples of (and identify) batch, semi-batch, continuous, steady, and transient processes

TEST YOURSELF

Under what modes of operation may batch or semi-batch process be run?

BPF: Define open system, closed system, adiabatic, isothermal

Further System Classifications

Now that we know the different types of systems (batch, semi-batch, continuous) and how they might be operated (steady, transient), it is useful to have one further layer of classification:

DEFINITION:

*A **closed system** is one where no mass moves across the boundaries. In terms of a flowchart, this means that there are no streams entering or leaving the closed system (in practice, this means that stuff goes in at the beginning and comes out only at the end).*

DEFINITION:

*An **open system** is one where mass does move across the boundaries. In practice, this means that stuff goes in or out at some point **during** the process (not simply at the beginning and/or ending).*

Open/closed tells us whether the system is isolated from its surroundings in terms of mass flow across the boundaries. Our last classifications have to do with whether a system is isolated from its surroundings in terms of *heat* flow and whether it changes temperature:

DEFINITION:

*An **adiabatic** system is one where no thermal energy (heat) moves across the boundaries (in practice, this is accomplished through the use of insulation, so this is often also called an "insulated" system).*

DEFINITION:

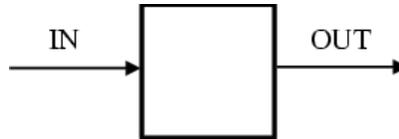
*An **isothermal** system stays at a single constant temperature with respect to time.*

OUTCOME:

Define open system, closed system, adiabatic, isothermal

BPF: Explain the origin and physical meaning of the General Mass Balance Equation

Material Balance Equation



DEFINITION

A **balance** is a method of accounting for something (here mass or material).

As we discussed when we defined balances earlier, the **general material balance** simply accounts for where things come/go and how their total number (or amount) changes. This led us to the following generic expression:

$$\text{IN} - \text{OUT} + \text{GENERATION} - \text{CONSUMPTION} = \text{ACCUMULATION}$$

where IN and OUT are the inputs and outputs to the system, respectively. In material and energy balances these will correspond to *process streams* and their contents. The GENERATION and CONSUMPTION accounted for ways in we could change the "stuff" in our system *without* flows in and out. In material and energy balances, this will correspond to chemical reactions.

In general, the types of systems that we have defined thus far (batch, continuous, etc.) are most easily handled by defining two alternate forms of this balance equation, in practice.

DEFINITION

A **differential balance** is a balance at one particular instant in time -- deals with rates (for mass balances: mass per time [kg/s]).

This type of balance is best suited for continuous processes and may be written more precisely in mathematical form as:

$$\frac{dM}{dt} = \dot{M}_I - \dot{M}_O + G - C$$

Where dM/dt denotes the rate of change of the material M (i.e., ACCUMULATION), G and C denote the rate of generation and consumption (respectively), and the overdots denote flowrates. (NOTE: all terms have units of mass/time.)

There are some special cases:

For steady state, ACCUMULATION=0, so

$$\text{IN} + \text{GENERATION} = \text{OUT} + \text{CONSUMPTION}$$

$$0 = \dot{M}_I - \dot{M}_O + G - C$$

For steady state, with no reaction

$$\text{IN} = \text{OUT}$$

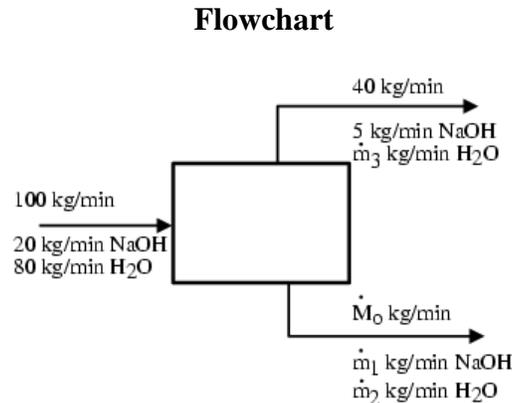
$$0 = \dot{M}_I - \dot{M}_O$$

EXAMPLE

Let's look at an example.

A process running at steady-state involves a 100 kg/min stream with a mixture of Water (80 kg/min) and Sodium Hydroxide (20 kg/min) being fed to a separator.

The mass flow of one of the two outlet streams (40 kg/min) is analyzed and found to contain 5 kg/min NaOH. Using differential balance equations, determine the mass flow rates of the remaining streams/components.



Write and simplify a balance equation on Water.

DEFINITION

An **integral balance** deals with the entire time of the process at once (so it uses amounts rather than rates: e.g., mass NOT mass/time).

This form of the equation is best suited for batch or semi-batch operation. A mathematical form for this equation can be derived by simply integrating the differential balance over the length of time the system is operating (i.e., from $t_{initial}$ to t_{final}). First we simply multiply both sides of the differential balance equation by dt to give:

$$dt \frac{dM}{dt} = dt \dot{M}_I - dt \dot{M}_O + dt G - dt C$$

which we can rearrange and then integrate:

$$\int_{t_{initial}}^{t_{final}} \frac{dM}{dt} dt = \int_{t_{initial}}^{t_{final}} \dot{M}_I dt - \int_{t_{initial}}^{t_{final}} \dot{M}_O dt + \int_{t_{initial}}^{t_{final}} G dt - \int_{t_{initial}}^{t_{final}} C dt$$

which ultimately leads to our final form of:

$$M_{t_{final}} - M_{t_{initial}} = \int_{t_{initial}}^{t_{final}} \dot{M}_I dt - \int_{t_{initial}}^{t_{final}} \dot{M}_O dt + \int_{t_{initial}}^{t_{final}} G dt - \int_{t_{initial}}^{t_{final}} C dt$$

There are some special cases:

For a closed system there is no input or output:

$$M_{t_{final}} - M_{t_{initial}} = \int_{t_{initial}}^{t_{final}} G dt - \int_{t_{initial}}^{t_{final}} C dt$$

For a closed system with no reaction (we get a really boring problem!):

$$M_{t_{final}} - M_{t_{initial}} = 0$$

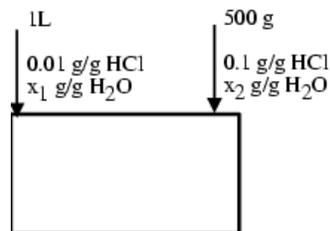
EXAMPLE

Let's look at an example.

The safety division of your company tells you that you are not allowed to dump acid that contains concentrations greater than a certain threshold (5% by mass) into the sink.

You have two solutions, one (1L) solution contains a mass fraction of 0.01 HCl in water and another (500 g) which has a mass fraction of 0.1 HCl. You wonder if you should combine the two and then dump them in the sink, or just cut your losses, dump the "legal" one, and properly dispose of the concentrated one. How would you determine which path to choose?

Flowchart



Can you write the proper integral balance?

OUTCOME:

Explain the origin and physical meaning of each of the terms in the General Mass Balance Equation

BPF: Explain the origin and physical meaning of the General Energy Balance Equation

Energy Balances

As with mass balances it is useful to start with our initial definition of a balance equation:

$$\text{IN} - \text{OUT} + \text{GENERATION} - \text{CONSUMPTION} = \text{ACCUMULATION}$$

Where IN and OUT correspond to energy flowing into and out of the system, respectively. In contrast to mass balances, however, energy is a *conserved* quantity (First Law of Thermodynamics) and therefore $\text{GENERATION} = \text{CONSUMPTION} = 0$! (We will see as we go that this is *also* true for total mass, and even for atoms, but *not* for specific molecular species). This gives us:

$$\text{IN} - \text{OUT} = \text{ACCUMULATION}$$

In order to finish this balance we need to look at exactly *how* energy can move IN and OUT of a system...

Also, as we did with mass balances, we need to start out with some definitions.

Types of Energy

DEFINITION:

Kinetic energy is energy due to the translational (or rotational) motion relative to some frame of reference.

DEFINITION:

Potential energy is energy due to something's position in a potential field (electromagnetic or gravitational, for example).

DEFINITION:

Internal energy is where we lump everyone else! (Thermal energy, chemical energy, etc.)

Each bit of mass within our balances will contain some amount of each of these forms of energy, so that we can write the *total* energy of some bit of mass as:

$$E_{\text{total}} = U + E_k + E_p$$

where U is the internal energy, E_k is the kinetic energy, and E_p is the potential energy.

How Energy Moves

Obviously, we can imagine that STUFF has energy (a hot potato, for example).

One way for the energy to move would be to move the entire potato! Therefore, like we had in mass balances we can have an IN-flow and OUT-flow in the system through moving mass. (Some potatoes may be hotter or colder, moving faster or slower, etc.)

In contrast to mass balances, however, we can also *change the energy that is in the potatoes already in the system*. Imagine putting a bucket of potatoes in the oven (we use heat to change the internal energy of the potatoes already in the bucket). Or perhaps we vigorously shake the bucket of potatoes; here, we convey mechanical (kinetic) energy right through the walls!

Energy Balance Equations

As with mass balances, energy balances will have an integral and differential form.

Recalling that our general energy balance equation looks like this:

IN - OUT = ACCUMULATION

We can start with our differential form by writing:

$$\frac{dE_{total}}{dt} = \dot{E}_{total\,in} - \dot{E}_{total\,out}$$

Recalling that total energy is given by:

$$E_{total} = U + E_k + E_p$$

we now simply need to account for the possibility of sticking stuff in an oven, or "shaking" it. We will denote the net flow of heat into the system as Q, and the net transfer of mechanical energy as W. The only catch is that we will consider a negative W to be going *into* the system, while a negative Q will be *coming out* of the system. This gives us:

General Differential Energy Balance

$$\frac{dU}{dt} + \frac{dE_k}{dt} + \frac{dE_p}{dt} = \dot{U}_{in} - \dot{U}_{out} + \dot{E}_{k\,in} - \dot{E}_{k\,out} + \dot{E}_{p\,in} - \dot{E}_{p\,out} + Q - W$$

For a steady state problem this reduces to:

$$\dot{U}_{out} - \dot{U}_{in} + \dot{E}_{k\,out} - \dot{E}_{k\,in} + \dot{E}_{p\,out} - \dot{E}_{p\,in} = Q - W$$

As we did with mass, we can integrate this to yield this integral form of the balance:

General Integral Energy Balance

$$\begin{aligned} & \dot{U}_{final} - \dot{U}_{initial} + \dot{E}_{k\,final} - \dot{E}_{k\,initial} + \dot{E}_{p\,final} - \dot{E}_{p\,initial} = \\ & \int_{t_{initial}}^{t_{final}} \dot{U}_{in} dt - \int_{t_{initial}}^{t_{final}} \dot{U}_{out} dt + \int_{t_{initial}}^{t_{final}} \dot{E}_{k\,in} dt - \int_{t_{initial}}^{t_{final}} \dot{E}_{k\,out} dt + \int_{t_{initial}}^{t_{final}} \dot{E}_{p\,in} dt - \int_{t_{initial}}^{t_{final}} \dot{E}_{p\,out} dt + \int_{t_{initial}}^{t_{final}} Q dt - \int_{t_{initial}}^{t_{final}} W dt \end{aligned}$$

which for a closed system simplifies to:

$$U_{final} - U_{initial} + E_{k\,final} - E_{k\,initial} + E_{p\,final} - E_{p\,initial} = \int_{t_{initial}}^{t_{final}} Q dt - \int_{t_{initial}}^{t_{final}} W dt$$

OUTCOME:

Explain the origin and physical meaning of each of the terms in the General Energy Balance Equation

BPF: Explain the difference between shaft work and flow work

Flow vs Shaft Work

In open systems (ones where material flows into and out of our process), we need to recall that takes energy (work) to make material flow! (Recall that you need to *squeeze* the toothpaste tube to get the stuff to flow out.)

The work term, therefore can be broken into a "shaft" component and a "flow" component:

DEFINITION:

Flow work is the energy necessary to cause flow in an open system.

DEFINITION:

Shaft work is any mechanical energy other than that necessary for flow. Typically this requires a stirrer or turbine (hence the name "shaft" work).

Mathematically, the differing types of work can be expressed as:

$$W = W_s + W_f = W_s + \Delta (PV)$$

The simplest way to account for this is to use enthalpy in open systems rather than energy since $H = U + PV$, in order to account for both internal energy and flow work at the same time.

OUTCOMES:

Explain the difference between shaft work and flow work

BPF: Simplify the appropriate form of the Energy Balance Equation

Closed Systems:

In a closed system, one typically uses an integral balance, based on internal energy. Furthermore, steady closed balances make no sense (since then *nothing at all* would happen) so we have the following practical forms:

Closed, unsteady:

$$U_{final} - U_{initial} + E_{k_{final}} - E_{k_{initial}} + E_{p_{final}} - E_{p_{initial}} = \int_{t_{initial}}^{t_{final}} Q dt - \int_{t_{initial}}^{t_{final}} W dt$$

if we consider Δ 's to denote changes from initial to final ($[]_{final} - []_{initial}$) and Q and W_s to be the heat and work over the "life" of the system, we will write this as:

$$\Delta U + \Delta E_k + \Delta E_p = Q - W$$

There are several "rules" to recall that can help in simplifying this further:

- U depends on chemical composition, phase, and temperature (only a little on pressure). *If no reactions, phase changes or temperature changes occur, the change in U is zero!* (except a little if the pressure changes a lot)
- Kinetic energy needs an acceleration (positive or negative) to change.
- Potential energy needs a change in position (height).
- If the system and surroundings are at the same T (or if we say that the system is (perfectly) insulated) then $Q = 0$ (the system is adiabatic).
- Work can only be done by moving parts (a compressive/expansion piston or rotating shaft) or by electrical or radiation energy.

Open Systems:

In an open system, we can use either an integral (for semi-batch problems) or a differential balance (for continuous problems). For semi-batch problems (by definition unsteady), we must use the general form of the integral balance (see the balances lesson). For continuous problems, we will use a modified form of the general balance which uses enthalpy, rather than energy (so only shaft work is explicitly included):

$$\frac{dH}{dt} + \frac{dE_k}{dt} + \frac{dE_p}{dt} = \dot{H}_{in} - \dot{H}_{out} + \dot{E}_{k_{in}} - \dot{E}_{k_{out}} + \dot{E}_{p_{in}} - \dot{E}_{p_{out}} + Q - W_s$$

For a steady problem (now using Δ 's to denote changes: $[]_{out} - []_{in}$):

$$\Delta \dot{H} + \Delta \dot{E}_k + \Delta \dot{E}_p = Q - W_s$$

OUTCOME:

Simplify the appropriate form of the Energy Balance Equation

TEST YOURSELF

*Write an equation for a steady state, open system that does not change height or speed.
What if it is also adiabatic?*

BPF: Draw and label a flowchart from a process description

Flowchart Development

We know what a flowchart is and what purpose it serves (organizing our thinking about a process) from the early part of this course. Let's look at a few flowchart *requirements* and then some conventions:

Requirements:

- Draw the process units and any streams connecting them
- Write the values and units of known stream variables
- Write each known stream flow and composition
- Assign algebraic symbols to unknown stream variables and put units on the unknowns!

There are three methods for conveying stream flows/compositions:

- Method 1: show a flow for each component
- Method 2: show a total flow, and fractional compositions of each component
- Method 3 (overkill): show a total flow and a flow for each component

Conventions:

- typically use uppercase letters for total flows (or masses) and lowercase for component flows (or masses)
- moles are typically denoted with "n" and masses with "m"
- overdots denote rates
- fractions are denoted as "x" in the liquid phase and "y" in the gas phase, "z" for the total fraction (including **both** liquid and gas)

Additional Flowchart Considerations

NOTE:

Flowcharts may be scaled.

It is not surprising that changing a flowchart from using units of lbm to kg should not make a difference to the validity of the flowchart. (unit conversions will not change whether the flowchart is balanced or not!)

With a little thinking then, it should be clear that changing the basis of calculation of a flowchart should not make a difference!

DEFINITION:

*A **basis** of calculation is the one stream whose amount (mass or moles) or flow rate (mass flow or molar flow) is chosen as the "least common denominator" for the problem (the units that you match everything to, as well as the scale you match everything to!).*

EXAMPLE:

For example: both of these expressions are true

$$60s + 120s = 180s$$

$$1 \text{ min} + 2 \text{ min} = 3 \text{ min}$$

Changing the units did not effect the truth of the statement. It should be equally clear that scaling up (multiplying by a number greater than 1) or scaling down (multiplying by a number less than 1) also makes little difference.

$$60s + 120s = 180s$$

$$6s + 12s = 18s \text{ (multiply by } 1/10\text{)}$$

$$120s + 240s = 360s \text{ (multiply by } 2\text{)}$$

OUTCOME

Draw and label a flowchart from a process description.

TEST YOURSELF

Let's try and work through an example.

Flowchart Example

From the following process description draw a flowchart that concisely summarizes each stage of the process (properly labeling all streams and species within those streams)

*An important, naturally-occurring chemical, A, is to be removed from its ore (composed of A and various insoluble other junk). 100 kg/hr of ore is fed to a **dissolution tank** where it is mixed with a stream of pure water, W, and a recycle stream. The tank is heated to 90C so that all of the A (but none of the other junk, J) dissolves, forming a saturated solution. The material exits the tank and is sent to a **filter (separator)** where all of the junk and a small portion of the (still saturated) solution is removed. Finally the remaining solution is fed to a **crystallizer** where it is cooled to 25C in order to form some solid A_s which is shipped off to be packaged and sold (some filtrate also leaves with the solid). The remaining filtrate, now saturated at 25C is recycled to the dissolution tank.*

Upon analyzing the products of from the filter and crystallizer, it is determined that the waste stream from the filter contains 40.0kg/hr of junk (J), 12 kg/hr of A, and 4 kg/hr of water (W) and that the final product stream from the crystallizer contains 42 kg/hr A_s , 6 kg/hr A_{aq} , and 6 kg/hr W.

OUTCOME

Draw and label a flowchart from a process description

TEST YOURSELF

Try another one.

Flowchart Example

From the following process description draw a flowchart that concisely summarizes each stage of the process (properly labeling all streams and species within those streams)

A distillation column is a device used to separate liquids of differing volatilities. The mixture is fed to the column and the more volatile material comes out as the "overhead" stream while the less volatile material comes out as the "bottoms".

In separating a three liquid system, one method is to use two distillation columns in series.

A mixture of three components A, B, and C are fed to a distillation column in equal amounts by mass at a rate of 100 kg/s. The overhead stream contains no C and all of the A (which comprises roughly 95 mass % of this stream's total flow). The bottom stream, flowing at 35 kg/s, is fed to a second column to separate B from C. The overhead from the second column contains essentially all B and the bottoms is roughly 5 mass % B.