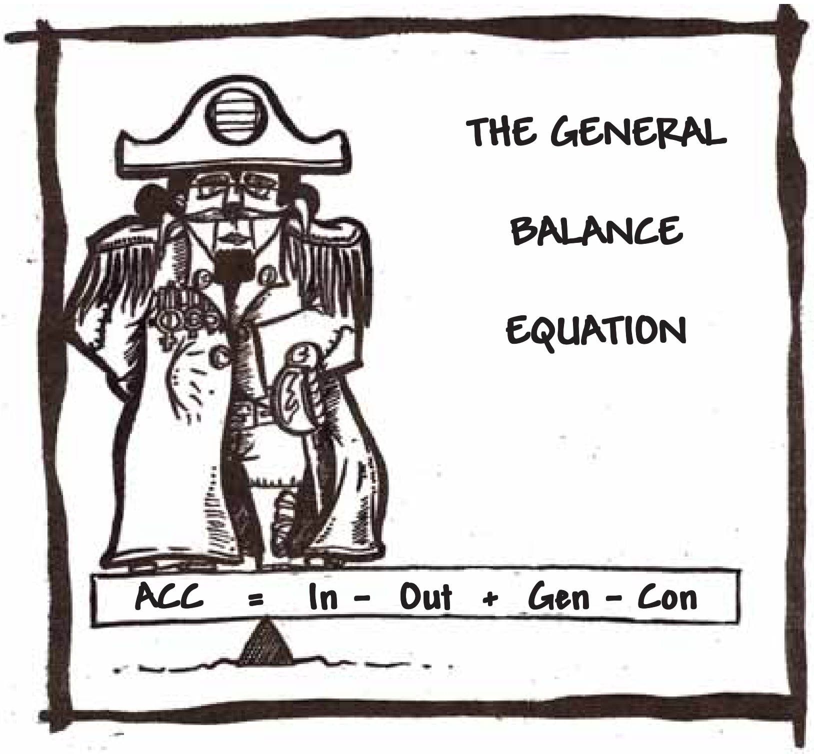
# CHAPTER ONE

# THE GENERAL BALANCE EQUATION



## THE GENERAL BALANCE

All material and energy (M&E) balance calculations are based on our experience that matter and energy may change its form, but it cannot appear from nor disappear to nothing. This observation is expressed mathematically in *Equation 1.01*, the *General Balance Equation.*

For a defined *system* and a specified *quantity:*

**Accumulation in system = Input to system – Output from system + Generation in system – Consumption in system** *Equation 1.01*

where:

Accumulation in system = [final amount of the quantity – initial amount of the quantity] inside the system boundary.
Input to system = amount of the quantity entering the system through the system boundary. (input)
Output from system = amount of the quantity leaving the system through the system boundary. (output)
Generation in system = amount of the quantity generated (i.e. formed) inside the system boundary. (source)
Consumption in system = amount of the quantity consumed (i.e. converted) inside the system boundary. (sink)

The general balance equation (*Equation 1.01*) is a powerful equation, which can be used in various ways to solve many practical problems. Once you understand *Equation 1.01* the calculation of M&E balances is simply a matter of bookkeeping.

The general balance equation (*Equation 1.01*) is the primary equation that is repeated throughout this text. In each chapter where it appears, the first number of this equation corresponds to the number of the chapter, so that it enters Chapter 4 as *Equation 4.01*, Chapter 5 as *Equation 5.01* and Chapter 7 as *Equation 7.01*.

Every time you apply *Equation 1.01*, you must begin by defining the *system* under consideration and the *quantity* of interest in the system. The *system* is a physical space, which is completely enclosed by a hypothetical envelope whose location exactly defines the extent of the system. The *quantity* may be any specified measurable (extensive[1]) property, such as the mass, moles,[2] volume or energy content of one or more components of the system. When *Equation 1.01* is applied to energy balances, the quantity also includes energy transfer across the system envelope as heat and/or work (see Chapter 5).

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[1] An extensive property is a property whose value is proportional to the amount of material.

[2] A *mole* is the amount of a substance containing the same number of "*elementary particles*" as there are atoms in 0.012 kg of carbon 12 (i.e. Avogadro's number = 6.028E23 particles). The number of moles in a given quantity of a molecular species (or element) is its mass divided by its molar mass, i.e. $n = m / M$. For molecular and ionic compounds in chemical processes (e.g. $H_2O$, $H_2$, $O_2$, $CH_4$, NaCl) the "*elementary particles*" are molecules. For unassociated elements and for ions the "*elementary particles*" are atoms (e.g. C, $Na^+$, $Cl^-$) or charged groups of atoms (e.g. $NH_4^+$, $ClO^-$). Refer to a basic chemistry text for more comprehensive information of atoms, ions, molecules and chemical bonding.

When you use the general balance equation it is best to begin with a conceptual diagram of the system, which clearly shows the complete system boundary plus the inputs and outputs of the system. *Figure 1.01* is an example of such a diagram. Note that:

- *Figure 1.01* is a two-dimensional representation of a real three-dimensional system
- The system has a closed boundary
- The system may have singular or multiple inputs and/or outputs

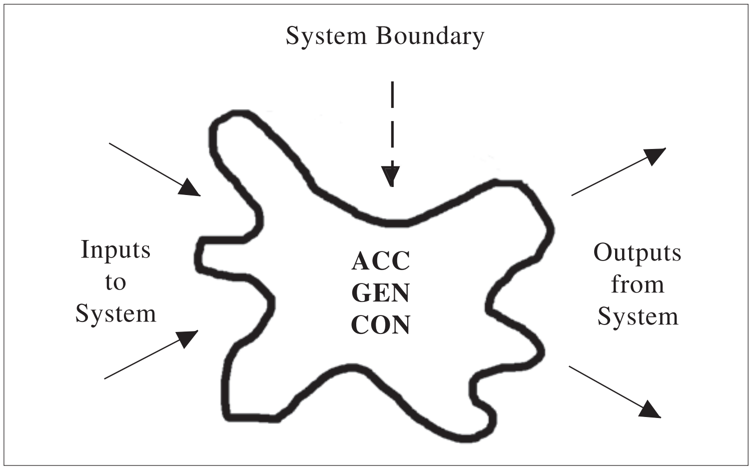

**Figure 1.01. Conceptual diagram of a system.**

## CONSERVED AND CHANGING QUANTITIES

The general balance equation (*Equation 1.01*) applies to any extensive quantity. However, when you use *Equation 1.01*, it is helpful to distinguish between quantities that are conserved and quantities that are not conserved. A conserved quantity is a quantity whose total amount is maintained constant and is understood to obey the *principle of conservation*, which states that such a quantity can be neither created nor destroyed. Alternatively, a conserved quantity is one whose total amount remains constant in an isolated system,[3] regardless of what changes occur inside the system.

For quantities that are conserved, the generation and consumption terms in *Equation 1.01* are both zero, whereas for quantities that are not conserved, either or both of the generation and consumption terms is not zero.

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[3] An isolated system is a hypothetical system that has zero interaction with its surroundings, i.e. zero transfer of material, heat, work, radiation, etc. across the boundary.

## MATERIAL AND ENERGY BALANCES

In general, material and energy are equivalent through *Equation 1.02*.

$$\mathbf{E = mc^2} \qquad \textit{Equation 1.02}$$

where:
E = energy J
m = mass (a.k.a. the rest mass) kg
c = velocity of light in vacuum = 3E8 $ms^{-1}$

In a system where material and energy are inter-converted, *Equation 1.01* can thus be written for the quantity ($mc^2$ + E) as:

| **Acc** | **=** | **In** | **–** | **Out** | **+** | **Gen** | **–** | **Con** | *Equation 1.03* |
|---|---|---|---|---|---|---|---|---|---|
| **($mc^2$ + E )** | | **($mc^2$ + E)** | | **($mc^2$ + E)** | | **($mc^2$ + E)** | | **($mc^2$ + E)** | |
| **in system** | | **to system** | | **from system** | | **in system** | | **in system** | |

The sum ($mc^2$ + E) is a conserved quantity, so the generation and consumption terms in *Equation 1.03* are zero. *Equation 1.03* thus reduces to *Equation 1.04*.

| **Accumulation of ($mc^2$ + E)** | **=** | **Input of ($mc^2$ + E)** | **–** | **Output of ($mc^2$ + E)** | *Equation 1.04* |
|---|---|---|---|---|---|
| **in system** | | **to system** | | **from system** | |

*Equation 1.04* is a mathematical statement of the general principle of conservation of matter and energy that applies to all systems within human knowledge.[4]

Excluding processes in nuclear engineering, nuclear physics, nuclear weapons and radiochemistry, systems on earth do not involve significant inter-conversion of mass and energy. In such non-nuclear systems, individual atomic species (i.e. elements) as well as the total mass and total energy are *independently* conserved quantities.

For individual atomic species in non-nuclear systems, *Equation 1.01* then reduces to *Equation 1.05*.

| **Accumulation of atoms** | **=** | **Input of atoms** | **–** | **Output of atoms** | *Equation 1.05* |
|---|---|---|---|---|---|
| **in system** | | **to system** | | **from system** | |

Also, *Equation 1.04* can be written as two separate and independent equations, one for total mass (*Equation 1.06*) and another for total energy (*Equation 1.07*).

| **Accumulation of mass** | **=** | **Input of mass** | **–** | **Output of mass** | *Equation 1.06* |
|---|---|---|---|---|---|
| **in system** | | **to system** | | **from system** | |

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[4] Modern cosmology may have more to say about the principle of conservation (see *Ref. 8*).

**Accumulation of energy in system = Input of energy to system – Output of energy from system** *Equation 1.07*

*Equation 1.05*, for the conservation of elements ≡ ATOM BALANCE
*Equation 1.06*, for the conservation of total mass ≡ MASS BALANCE
*Equation 1.07*, for the conservation of total energy ≡ ENERGY BALANCE

The word "total" is used here to ensure that *Equations 1.06* and *1.07* are not applied to the mass or energy associated with only part of the system (e.g. a single species or form of energy) — which may not be a conserved quantity.

*Equations 1.05, 1.06* and *1.07* are **special cases of *Equation 1.01*** that apply to conserved quantities. The strength of *Equation 1.01* is that it can also be applied to quantities that are not conserved. The generation and consumption terms of *Equation 1.01* then account for changes in the amounts of non-conserved quantities in the system (see *Ref. 7*).

Some of the quantities that can be the subject of *Equation 1.01*, applied to non-nuclear proceses, are:

Elements : Conserved — *Equation 1.05* — Atom balance
Total mass : Conserved — *Equation 1.06* — Total mass balance
Total energy : Conserved — *Equation 1.07* — Total energy balance
Momentum : Conserved — Momentum balance
Moles : Conserved in systems without chemical reaction.
Not necessarily conserved in systems with chemical reaction
Enthalpy : Not necessarily conserved
Entropy : Not necessarily conserved
Volume : Not necessarily conserved

*Examples 1.01* and *1.02* show how *Equation 1.01* is applied respectively to a conserved quantity and to a non-conserved quantity.

### *EXAMPLE 1.01 Material balance on water in a reservoir.*

A water reservoir initially contains 100 tonne of water. Over a period of time 60 tonne of water flow into the reservoir, 20 tonne of water flow out of the reservoir and 3 tonne of water are lost from the reservoir by evaporation. Water is not involved in any chemical reactions in the reservoir.

***Problem:***

What is the amount of water in the reservoir at the end of the period of time? [Answer in tonnes of water]

***Solution:***

Define the system = the reservoir

Specify the quantity = mass of water [conserved quantity]

Write the balance equation:

ACC of water in system = IN of water to system − OUT of water from system + GEN of water in system − CON of water in system

Interpret the terms:

Accumulation of water in system = final mass of water in system − initial mass of water in system = unknown = X

Input of water to system = 60 tonne

Output of water from system = 20 (flow) + 3 (evaporation) = 23 tonne

Generation of water in system = 0 (water is conserved) tonne

Consumption of water in system = 0 (water is conserved) tonne

Substitute values for each term into the general balance equation

$X = 60 - (20 + 3) + 0 - 0$

Solve the balance equation for the unknown.

$X = 37$ tonne

Final mass of water in system

= Initial mass of water in system + X = 100 + 37 = **<u>137 tonne</u>**

***EXAMPLE 1.02 Material balance on the population of a country.***

A country had a population of 10 million people in 1900 AD. Over the period from 1900 to 2000 AD, 4 million people immigrated into the country, 2 million people emigrated from the country, 5 million people were born in the country and 3 million people died in the country.

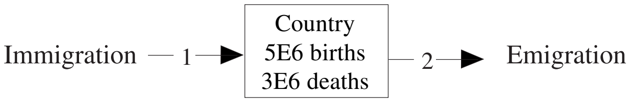
***Problem:***

What is the population of the country in the year 2000 AD?

***Solution:***

Define the system = country

Specify the quantity = number of people [a non-conserved quantity]



Write the balance equation:

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ACC of people in system | = | IN of people to system | – | OUT of people from system | + | GEN of people in system | – | CON of people in system |

Interpret the terms:

Accumulation = Final no. of people in system – Initial no.of people in system = unknown = X

| | | | | |
|---|---|---|---|---|
| Input of people to system | = | immigration | = | 4 million people |
| Output of people from system | = | emigration | = | 2 million people |
| Generation of people in system | = | born | = | 5 million people |
| Consumption of people in system | = | died | = | 3 million people |

Substitute values into the general balance equation

$X = 4 - 2 + 5 - 3 = 4$ million people

Final number of people in 2000 AD:

Initial no. of people in 1900 + X = 10 + 4 = **<u>14 million people</u>**

*Example 1.03* shows a slightly more difficult case of a non-conserved quantity involving chemical reaction stoichiometry.

***EXAMPLE 1.03 Material balance on carbon dioxide from an internal combustion engine.***

An automobile driven by an internal combustion engine burns 10 kmol of gasoline[5] consisting of 100% octane ($C_8H_{18}$) and converts it completely to carbon dioxide and water vapour by a combustion reaction, whose stoichiometric equation is:

$$2C_8H_{18} + 25O_2 \rightarrow 16\,CO_2 + 18H_2O \qquad \textit{Reaction 1}$$

All $CO_2$ and $H_2O$ produced in the reaction is discharged to the atmosphere via the engine's exhaust pipe (i.e. zero accumulation).

Assume $CO_2$ content of input combustion air = zero

***Problem:*** What is the amount of carbon dioxide discharged to the atmosphere from 10 kmol octane? [Answer in kg of $CO_2$]

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[5] kmol ≡ kilomole ≡ molar mass (molecular weight) expressed as kilograms.
1 kmol $C_8H_{18}$ = (12.01)(8) + (1.008)(18) = 114.22 kg = 162 litre = 43 US gallons, i.e. about 3 tanks of gasoline (a.k.a. petrol) for a family car.

***Solution:*** First note that the amount (mass or moles) of $CO_2$ is not a conserved quantity. Chemical reactions involve the consumption of reactant species and the generation of product species, so that no species appearing in the stoichiometric equation is conserved when a reaction occurs.

Define the system = automobile internal combustion engine

Specify the quantity = mol (kmol) of $CO_2$ [mole quantities give the simplest calculations for chemical reactions]

Write the balance equation:

$$\begin{array}{ccccccccc}\text{ACC of } CO_2 & = & \text{IN of } CO_2 & - & \text{OUT of } CO_2 & + & \text{GEN of } CO_2 & - & \text{CON of } CO_2 \\ \text{in system} & & \text{to system} & & \text{from system} & & \text{in system} & & \text{in system}\end{array}$$

Interpret the terms:

| | | | |
|---|---|---|---|
| Accumulation of $CO_2$ in system | = 0 | kmol | (all $CO_2$ is discharged) |
| Input of $CO_2$ to system | = 0 | kmol | (zero $CO_2$ enters engine) |
| Output of $CO_2$ from system | = unknown = X | kmol | |
| Generation of $CO_2$ in system | = (16/2)(consumption of $C_8H_{18}$ in system) = (16/2)(10 kmol) | | |
| | = 80 | kmol | (from stoichiometry of *Reaction 1*) |
| Consumption of $CO_2$ in system | = 0 | kmol | ($CO_2$ is a product, not a reactant) |

Substitute values for each term into the general balance equation.

$$0 = 0 - X + 80 - 0$$

Solve the balance equation for the unknown "X".

X = 80 kmol $CO_2$ discharged to atmosphere

$\equiv$ (80 kmol)(((1)(12.01) + (2)(16.00)) kg/kmol) = $\underline{\mathbf{3521\ kg\ CO_2}}$

## FORMS OF THE GENERAL BALANCE EQUATION

There are several forms of the general balance equation (*Equation 1.01*), with each form suited to a specific class of problem.

First, for convenience, *Equation 1.01* is usually written in shorthand as:

**ACC = IN – OUT + GEN – CON** (see *Equation 1.01*)

where:

| | | |
|---|---|---|
| ACC | = Accumulation of specified quantity in system = (Final amount – Initial amount) of quantity in system. | |
| IN | = Input of specified quantity to system | (input) |
| OUT | = Output of specified quantity from system | (output) |
| GEN | = Generation of specified quantity in system | (source) |
| CON | = Consumption of specified quantity in system | (sink) |

As written above *Equation 1.01* is an *integral balance* suited to deal with the *integrated (total) amounts* of the specified quantity in each of the five terms over a period of time from the initial to the final state of the system. The integral balance equation can be used for any system with any process but is limited to seeing only the total changes occurring between the initial and final states of the system. Calculations with the integral balance require the solution of algebraic equations.

When *Equation 1.01* is differentiated with respect to (w.r.t.) time it becomes a *differential balance* equation (*Equation 1.08*), with each term representing a RATE of change of the specified quantity with respect to time, i.e.

**Rate ACC = Rate IN – Rate OUT + Rate GEN – Rate CON** *Equation 1.08*

where:

| | | |
|---|---|---|
| Rate ACC | = Rate of accumulation of specified quantity in system, | w.r.t. time |
| Rate IN | = Rate of input of specified quantity to system, | w.r.t. time |
| Rate OUT | = Rate of output of specified quantity from system, | w.r.t. time |
| Rate GEN | = Rate of generation of specified quantity in system, | w.r.t. time |
| Rate CON | = Rate of consumption of specified quantity in system, | w.r.t. time |

*Equation 1.08* is suited to deal with both closed systems and open systems involving unsteady-state processes, as well as with open systems involving steady-state processes. These terms are defined below in "Class of Problem".

The differential balance equation is more versatile than the integral balance equation because it can trace changes in the system over time. Application of the differential balance to unsteady-state processes requires knowledge of calculus to solve differential equations. For steady-state processes, the differential equation(s) can be simplified and solved as algebraic equation(s).

## CLASS OF PROBLEM

Practical problems are classified according to the type of system and the nature of the process occurring in the system, as follows:

| | | | |
|---|---|---|---|
| **Closed system** | Zero material* is transferred in or out of the system [during the time period of interest]. | | |
| [Controlled mass] | i.e. in the material balance equation: | IN = OUT = 0 | |
| | A process occurring in a closed system is called a BATCH process. | | |
| **Open system** | Material is transferred in and/or out of the system. | | |
| [Controlled volume] | i.e. in the material balance equation: | IN $\neq$ 0 and/or OUT $\neq$ 0 | |
| | A process occurring in an open system is called a CONTINUOUS process. | | |
| **Steady-state process** | A process in which all conditions are invariant with time. | | |
| | i.e. at steady-state: | Rate ACC = 0 | for all quantities. |
| **Unsteady-state process** | A process in which one or more conditions vary with time [these are *transient* conditions], i.e. at unsteady-state: | Rate ACC $\neq$ 0 | for one or more quantities. |

* *Energy can be transferred in and/or out of both closed and open systems.*

From these generalisations we can write balance equations for special cases that occur frequently in practical problems.

| | | |
|---|---|---|
| Differential material[6] balance on a closed system: | **Rate ACC = Rate GEN – Rate CON** | *Equation 1.09* |
| Differential total mass balance on a closed system: | **Rate ACC = 0** | *Equation 1.10* |
| Differential material balance on an open system at steady-state: | **0 = Rate IN – Rate OUT + Rate GEN – Rate CON** | *Equation 1.11* |
| Differential total mass balance on an open system: | **Rate ACC = Rate IN – Rate OUT** | *Equation 1.12* |
| Differential total mass balance on open system at steady-state: | **0 = Rate IN – Rate OUT** | *Equation 1.13* |
| Differential total energy balance on a closed or an open system: | **Rate ACC = Rate IN – Rate OUT** | *Equation 1.14* |
| Differential total energy balance at steady-state: | **0 = Rate IN – Rate OUT** | *Equation 1.15* |

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[6] Note that "material" and "mass" are not synomymous terms. Material may change its form, but the total mass is constant (in non-nuclear processes).

*Equations 1.09* to *1.15* can be applied either as differential balances or as integral balances with the terms integrated over time.

A powerful feature of *Equation 1.01* is your freedom to define both the *system* and the *quantity* to suit the problem at hand. For example, if you are working on global warming, the *system* could be a raindrop, a tree, a cloud, an ocean or the whole earth with its atmosphere, while the *quantity* may be the mass (or moles) of carbon dioxide, the mass (or moles) water vapour or the energy content associated with the system. If you are working on a slow release drug, the *system* could be a single cell, an organ or the whole human body, while the *quantity* may be the mass of the drug or its metabolic product, etc.

For an industrial chemical process (the focus of this text[7]) the *system* could be defined as, for example:

- a single molecule
- a microelement of fluid
- a bubble of gas, drop of liquid or particle of solid
- a section of a process unit (e.g. a tube in a heat exchanger, a plate in a distillation column, etc.)
- a complete process unit (e.g. a heat exchanger, an evaporator, a reactor, etc.)
- part of a process plant including several process units and piping
- a complete process plant
- a complete process plant plus the surrounding environment

In an industrial chemical process the *quantity* of interest may be, for example:

- total mass or total moles of all species
- mass or moles of any single species
- mass or atoms of any single element
- total energy

Other quantities that may be used in process calculations are, for example:

- total mass plus energy of all species (nuclear processes)
- one form of energy (e.g. internal energy, kinetic energy, potential energy)
- volume of one or more components
- enthalpy
- entropy [not treated in this text]
- momentum [not treated in this text]

The choice of both the *system* and the *quantity* are major decisions that you must make when beginning an M&E balance calculation. These choices are usually obvious but sometimes they are not. You should always give these choices careful consideration because they will determine the degree of difficulty you encounter in solving the problem.

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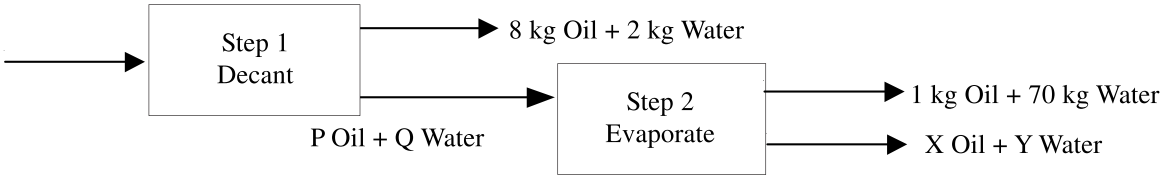
[7] The techniques described here for an industrial chemical process can be applied to any system in which you are interested.

*Examples 1.04* and *1.05* show that selection of the *system* and the *quantity* can affect the ease of solution of M&E balance problems. *Example 1.04* is a multi-stage balance problem that can be solved either by stage-wise calculations or by an overall balance. Solution A shows the stage-wise approach while solution B shows the more efficient solution obtained by defining an overall system that includes all the process steps inside a single envelope. In *Example 1.05* you can see how a relatively complex multi-stage problem involving chemical reactions can be reduced to one overall balance on the quantity of a single element (carbon). Such atom balances (on one or more elements) are handy for resolving many material balance problems. However there are other more complex problems represented in Chapter 4 whose solution requires stage-wise balances on each chemical species over every process unit.

***EXAMPLE 1.04 Material balance on a two-stage separation process.***

A 100 kg initial mixture of oil and water contains 10 kg oil + 90 kg water. The mixture is separated in two steps.[8]

**Step 1**. 8 kg oil with 2 kg water is removed by decantation. **Step 2.** 1 kg oil with 70 kg water is removed by evaporation.



***Problem:*** Find the amounts of oil and water in the final mixture (i.e. X kg oil + Y kg water).

***Solution A:*** [Stepwise balances]

**Step 1:** Define the system = Decanter (an open system)
Specify the quantities = Mass of oil, mass of water

Write the integral balance equation: **ACC = IN – OUT + GEN – CON**

**For the oil:**
ACC = Final oil in system – Initial oil in system = 0
IN = 10 kg
OUT = 8 + P kg
GEN = 0 kg [Oil is conserved]
CON = 0 kg

**For the water:**
ACC = Final water in system – Initial water in system = 0
IN = 90 kg
OUT = 2 + Q kg
GEN = 0 kg [Water is conserved]
CON = 0 kg

Mass balance on oil: ACC = 0 = 10 – (8 + P) + 0 – 0 P = 2 kg oil
Mass balance on water: ACC = 0 = 90 – (2 + Q) + 0 – 0 Q = 88 kg water

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[8] Assumes the decanter and the evaporator are empty before and after the operation; i.e. accumulation = 0.

**Step 2:** Define the system = Evaporator (an open system)
Specify the quantities = Mass of oil, mass of water

Write the integral balance equation: **ACC = IN – OUT + GEN – CON**

| **For the oil:** | **For the water:** |
|---|---|
| ACC = Final oil in system – Initial oil in system = 0 | ACC = Final water in system – Initial water in system = 0 |
| IN = 2 kg | IN = 88 kg |
| OUT = 1 + X kg | OUT = 70 + Y kg |
| GEN = 0 kg [Oil is conserved] | GEN = 0 kg [Water is conserved] |
| CON = 0 kg | CON = 0 kg |

Mass balance on oil: ACC = 0 = 2 – (1 + X) + 0 – 0 **X = 1 kg oil**
Mass balance on water: ACC = 0 = 88 – (70 + Y) + 0 – 0 **Y = 18 kg water**

***Solution B:*** [Overall balance]
Define the system = Decanter + evaporator (i.e. overall process)
Specify the quantities = Mass of oil, mass of water

Write the integral balance equation: **ACC = IN – OUT + GEN – CON**

| **For the oil:** | **For the water:** |
|---|---|
| ACC = Final oil in system – Initial oil in system = 0 | ACC = Final water in system – Initial water in system = 0 |
| IN = 10 kg | IN = 90 kg |
| OUT = 8 + 1 + X kg | OUT = 2 + 70 + Y kg |
| GEN = 0 kg [Oil is conserved] | GEN = 0 kg [Water is conserved] |
| CON = 0 kg | CON = 0 kg |

Mass balance on oil: ACC = 0 = 10 – (8 + 1 + X) + 0 – 0 **X = 1 kg oil**
Mass balance on water: ACC = 0 = 90 – (2 + 70 + Y) + 0 – 0 **Y = 18 kg water**

*Example 1.04* shows that (when the intermediate conditions are not required) the overall balance gives the most efficient solution.

***EXAMPLE 1.05 Material balance on carbon dioxide from a direct methanol fuel cell.***

Methanol ($CH_3OH$) is used as the fuel in an automobile engine based on a direct methanol fuel cell. The fuel supply for one tank of methanol is produced from 10 kmol[9] of natural gas (methane, $CH_4$) by the following process:

1. Eight kmol of $CH_4$ reacts completely with water (steam) to produce CO and $H_2$ by the stoichiometry of *Reaction 1.*

   $CH_4 + H_2O \rightarrow CO + 3H_2$ *Reaction 1*

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[9] 10 kmol $CH_4 \equiv$ (10 kmol)(16.04 kg/kmol) = 160.4 kg $CH_4$.

2. Two kmol of $CH_4$ is burned in *Reaction 2* to supply heat to drive *Reaction 1*.

   $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ ($CO_2$ to atmosphere) *Reaction 2*

3. One-third of the $H_2$ from *Reaction 1* is converted to water by *Reaction 3*.

   $2H_2 + O_2 \rightarrow 2H_2O$ *Reaction 3*

4. The remaining CO and $H_2$ are converted to $CH_3OH$ by *Reaction 4*.

   $CO + 2H_2 \rightarrow CH_3OH$ *Reaction 4*

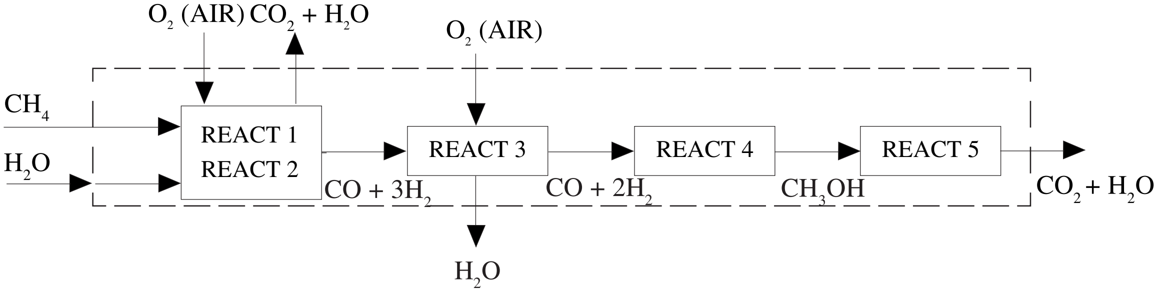
5. The methanol is subsequently completely converted to $CO_2$ and $H_2O$ by the net *Reaction 5*, which occurs in the fuel cell to produce power for the automobile.

   $CH_3OH + 1.5\,O_2 \rightarrow CO_2 + 2H_2O$ ($CO_2$ to atmosphere) *Reaction 5*

***Problem:*** Find the total amount of $CO_2$ released to the atmosphere from these operations, starting with the 10 kmol of $CH_4$. Assume zero accumulation of material in all the process steps. [kg $CO_2$]

***Solution:*** We can define each of the 5 reaction steps as a separate system and trace the production of $CO_2$ through the sequence of operations, or we can define any combination of steps as the system (provided it is enclosed by a complete envelope). In this case it is most efficient to define the system to include all 5 reaction steps and carry out an overall atom balance on the open system.

Define the system = the overall process of 5 reaction steps [closed envelope, shown by broken line].
Specify the quantity = moles (kmol) of the element carbon [contained in various compounds].
Write the integral balance equation: **ACC = IN – OUT + GEN – CON**



ACC = Final C in system – Initial C in system = 0 (i.e. zero accumulation)
IN = (10 kmol $CH_4$)(1 kmol C/kmol $CH_4$) = 10 kmol C
OUT = (X kmol $CO_2$)(1 kmol C/kmol $CO_2$) = X kmol C
GEN = 0 [carbon is conserved]
CON = 0 [carbon is conserved]

0 = 10 – X + 0 – 0
X = 10 kmol $CO_2$ ≡ (10 kmol)(44 kg/kmol) **= 440 kg $CO_2$ total to atmosphere**

*Example 1.06* shows the solution of a material balance using a differential balance on an open system and also illustrates how a problem involving chemical reaction can be solved either by mole balances from the reaction stoichiometry or by atom balances on selected elements. You should note here that for a single reaction the atom balance method is simpler than the mole balance because the atom balance does not need to use the reaction stoichiometric equation. In more complex cases, such as those involving reactions with incomplete conversion and/or where the specified elements appear in several products, the mole balance is often the prefered method of solution.

***EXAMPLE 1.06 Material balance on water vapour from a jet engine.***

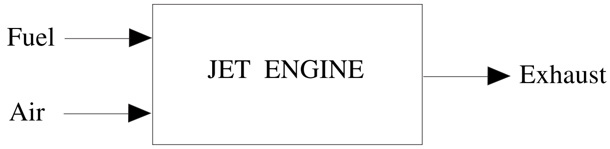
Water vapour trails from jet planes are known to initiate cloud formation and are one suspected cause of global climate change.

A jet engine burns kerosene fuel ($C_{14}H_{30}$) at the steady rate of 1584 kg/h.

The fuel undergoes complete combustion to $CO_2$ and $H_2O$.

***Problem:*** Calculate the flow of water vapour in the engine exhaust stream. [kg/h]

***Solution A:*** (Mole balance) Define the system = jet engine (an open system)
Specify the quantity = moles (kmol) of water



Write the reaction stoichiometry:

$$2C_{14}H_{30} + 43O_2 \rightarrow 28CO_2 + 30H_2O \qquad \textit{Reaction 1}$$

Let X = flow of water in engine exhaust. [kmol/h]

Write the differential material balance:

**Rate ACC = Rate IN – Rate OUT + Rate GEN – Rate CON**

Rate ACC = 0 (steady-state)
Rate IN = 0
Rate OUT = X
Rate GEN = (15 kmol $H_2O$/kmol $C_{14}H_{30}$)(1584 kg $C_{14}H_{30}$/h)/(198 kg $C_{14}H_{30}$/kmol $C_{14}H_{30}$) = 120 kmol/h $H_2O$
Rate CON = 0

0 = 0 – X + 120 – 0 X = 120 kmol $H_2O$ /h = (120 kmol/h)(18 kg/kmol) = **<u>2160 kg/h $H_2O$</u>**

***NOTE:*** Nitrogen ($N_2$) in the air is assumed to pass unchanged through the combustion process. In reality a small fraction of the nitrogen is converted to nitrogen oxides, NO and $NO_2$.

***Solution B:*** (Atom balance) Define the system = jet engine
Specify the quantity = moles (kmol) of hydrogen atoms i.e: hydrogen as $H_1$

Let X = flow of water in engine exhaust. [kmol/h]

Write the differential material balance:

**Rate ACC = Rate IN – Rate OUT + Rate GEN – Rate CON**

Rate ACC = 0 (steady-state)
Rate IN = (1584 kg/h $C_{14}H_{30}$)/(198 kg $C_{14}H_{30}$/kmol $C_{14}H_{30}$)(30 kmol $H_1$/kmol $C_{14}H_{30}$) = 240 kmol/h $H_1$
Rate OUT = (X kmol/h $H_2O$)(2 kmol $H_1$ / kmol $H_2O$) = 2X kmol/h $H_1$
Rate GEN = Rate CON = 0 (atoms are conserved)

0 = 240 – 2X + 0 – 0
X = 120 kmol $H_2O$ /h = (120 kmol/h)(18 kg/kmol) = **<u>2160 kg/h $H_2O$</u>**

Differential balances on closed systems and unsteady-state open systems require solution by calculus and are not considered until Chapter 7.

## SUMMARY

**[1]** The general balance equation (GBE) is the key to material and energy (M&E) balance problems.

The GBE can be used in integral or in differential form.

For a defined *system* and a specified *quantity:*

Integral form of GBE

**ACC = IN – OUT + GEN – CON** (see *Equation 1.01*)

Differential form of GBE

**Rate ACC = Rate IN – Rate OUT + Rate GEN – Rate CON** (see *Equation 1.08*)

**[2]** Always begin work with the GBE by defining the system (a closed envelope) and specifying the quantity of interest. Take care here to avoid ambiguity. *Ambiguity is the mother of confusion.*

**[3]** The choice of both *system* and *quantity* in the GBE determines the ease of solution of M&E balance problems. The *system* can range from a sub-micron feature to a whole planet and beyond, or from a single unit in a multi-stage sequence to the overall operation. The *quantity* may be any specified measurable (extensive) property, such as the mass, moles, volume or energy of one or more components of the system.

**[4]** The GBE applies to both conserved and non-conserved quantities.
For conserved quantities: GEN = CON = 0
For non-conserved quantities: GEN and/or CON ≠ 0

**[5]** In non-nuclear processes the individual atomic species (elements) as well as both total mass and total energy are independently conserved quantities, for which the GBE's simplify to:

Atom (element) balance:

**Atoms ACC = Atoms IN – Atoms OUT** (see *Equation 1.05*)

Total mass balance:

**Mass ACC = Mass IN – Mass OUT** (see *Equation 1.06*)

Total energy balance:

**Energy ACC = Energy IN – Energy OUT** (see *Equation 1.07*)

**[6]** M&E balance problems are broadly classified by system and process as:

| | | |
|---|---|---|
| Closed system: | Material IN = Material OUT = 0 | [Controlled mass] |
| Open system: | Material IN and/or Material OUT ≠ 0 | [Controlled volume] |
| Batch process: | Process occurring in a closed system. | |
| Continuous process: | Process occurring in an open system. | |
| Steady-state process: | Invariant with time.<br>Rate ACC = 0 for all quantities | |
| Unsteady-state process: | Variant with time.<br>RateACC ≠ 0 for one or more quantities | |

**[7]** Energy may be transferred in and/or out of both closed and open systems.

**[8]** The calculation of an M&E balance can sometimes be simplified by choosing a conserved quantity and/or by making an overall balance on a multi-unit sequence. Always check these options before starting a more detailed analysis.

**[9]** *Examples 1.01* to *1.06* are simple material balance problems that illustrate the concepts of the GBE. Subsequent chapters will show how the GBE is used to solve more complex material and energy problems, with emphasis on practical chemical processing.

## FURTHER READING

[1] R. M. Felder and R. W. Rousseau, *Elementary Principles of Chemical Processes*, John Wiley & Sons, New York, 2000.

[2] D. M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, Prentice Hall, Englewood Cliffs, 1989.

[3] O. A. Hougen, K. M. Watson and R. A. Ragatz, *Chemical Process Principles*, John Wiley, New York, 1954.

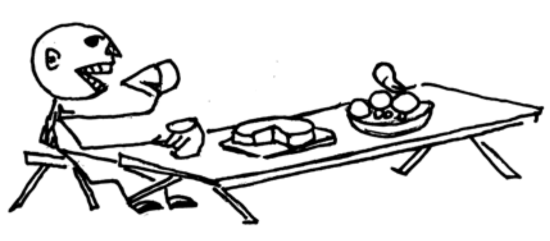
[4] P. M. Doran, *Bioprocess Engineering Principles*, Academic Press, San Diego, 1995.

[5] G. V. Reklaitis, *Material and Energy Balances,* John Wiley & Sons, New York, 1983.

[6] R. K. Sinnot, *Chemical Engineering Design*, Butterworth-Heinmann, Oxford, 1999.

[7] S. I. Sandler, *Chemical and Engineering Thermodynamics*, John Wiley & Sons, New York, 1999.

[8] S. W. Hawking, *The Theory of Everything — The Origin and Fate of the Universe*, New Millenium Press, Beverly Hills, 2002.



MATERIAL TRANSFER ACROSS A SYSTEM BOUNDARY