



Mass Balance of a component in Transient State

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1 Abstract

In this paper, we will present an application of the transient state of **mass balances** for the purposes of predicting the variation in concentration of a component in a system over time. The equation resulting from the application of the balances will be validated with experimentally obtained data. In this way, we want to highlight the usefulness of the balances to predict what happens in a process and thus avoid experimental set-up.

First of all, we will familiarize ourselves with the general structure of the balances (Figure 1):

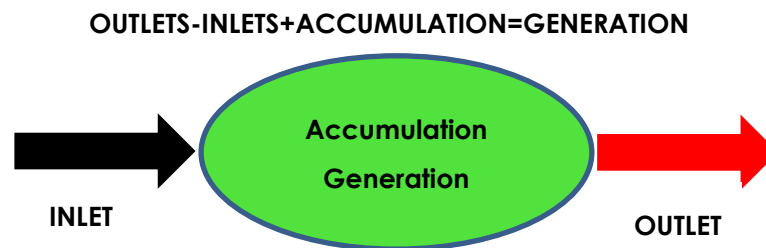


Figure 1. Representation of the terms of the general equation of balances in a system. With:

- **Inlet/Outlet:** Being that which crosses the boundaries of the system.
- **Accumulation:** Being the variation in a given time of that which is within the system.
- **Generation:** Being that which appears or disappears within the boundaries of the system without initially being present or having been transferred across the boundaries.

It will not always be necessary to consider all the terms of the general equation of the balances. In the event that there is no appearance or disappearance of any chemical species in the system, we will not consider the generation. However, if *the time variable affects its physicochemical properties*, **accumulation** will have to be considered. In the latter case, we will say that the system is in a **non-stationary or transient state**.

2. Introduction

In order to successfully predict the necessary quantities of the different components required to make a food or drug formulation based on its composition, **mass balances** are used (Tarrazó, 2002; Tarrazó and Sanjuán, 2005). These mathematical tools consider the different *mass flow rates of input* (m_e) *and output* (m_s) to a system expressed as kg of total mass or of a specific component per unit of time. In addition, the term of *accumulation* is also considered, which represents the variation in the amount of total mass (dM/dt) or of a component i (dx_i/dt) as a function of time. Finally, in situations in which chemical species appear or disappear during the operation, we will take into account a term of generation of this species (g_i). To be able to operate with the balances, we will apply **the Law of the Conservation of Mass, the Lomonosov-Lavoisier Law or the First Law of Thermodynamics**, which establishes that mass and energy are neither created nor destroyed, but transformed (Figure 2).



Figure 2. Example of the law of conservation of mass (Rotary, 2020; Marcos, 2016).

3 Objectives

Once you have carefully read this document, you will be able to apply mass balances for the purposes of predicting the concentration of a given component in a given stream of an industrial process.

4. Development

When applying mass balances, we must begin by graphically representing our case study. To do this, we will use a **flow diagram** in which each of the stages of the process is represented in blocks in which arrows enter or leave indicating the input or output of the different streams involved in the process. Then, you will apply the balances of both total mass and the component we want to predict. Finally, you will validate the equation obtained with experimental data.

4.1 Theoretical Case study

As the best way to see how to work with balances is to use them in a **practical case**, let us consider one. *Let us assume an industrial process consisting of an agitated tank containing an initial volume (V_0) of salt water solution with a concentration c_0 expressed in grams of salt per litre of solution (g/L). At a certain time, a stream of pure water with a volumetric flow rate q_1 (L/min) is inserted into this tank and, simultaneously, a stream with a volumetric flow rate similar to that of the inlet is extracted ($q_2=q_1$). **What will be the mathematical function relating the salt concentration in the tank with time?***

To answer the above question let's look at the steps to follow:

1. Represent all the streams in a flowchart.

From the data provided in the process to be studied, we will be able to know which streams are involved in the process and we will identify them with a number. In this example we have inlet current 1 and outlet current 2 expressed in volumetric units. In addition, we know that inlet stream 1 has a volumetric flow rate q_1 which is identical to outlet stream q_2 . On the other hand, we know the initial salt concentration of the reservoir solution (c_0), expressed in grams of salt per litre of solution (Figure 3).

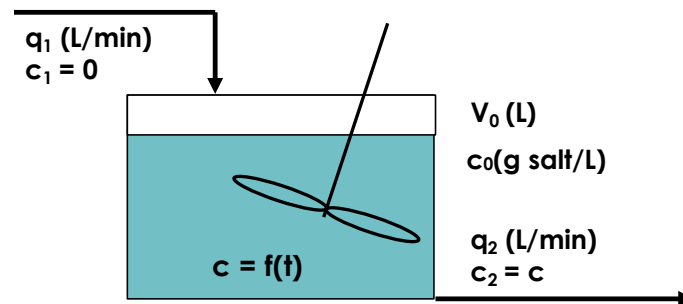


Figure 3. Theoretical flow diagram of a tank with a salt solution in which a stream of unsalted water enters and another stream of solution flows out simultaneously, diluting over time.

2. Propose the balances of total mass and of as many components as are considered to be linearly independent.

As we have seen in the previous section (Figure 2), **mass is what is conserved**, so we are going to consider total mass balances or balances of the component with which we are working. In this sense, in the application of mass balances it is usual to work with mass flow rates (m , kg per unit of time) and with the composition of each component (i), expressed in mass fractions (x_i , kilograms of component i with respect to total kilograms). Thus, from the general equation of the balances given in the summary of this learning object, the following mathematical expressions are obtained:

TOTAL MASS, BALANCE (BMT) (total kilograms):

$$\sum m_s - \sum m_e + \frac{dM}{dt} = G$$

BALANCE OF EACH COMPONENT (BC) (kilograms of each component):

$$\sum x_{is} m_s - \sum x_{ie} m_e + x_i \frac{dM}{dt} + M \frac{dx_i}{dt} = g_i$$

In the present case we know that the volume variation in the system over time will be zero, since the volume flow rate of the inlet stream is equal to the volume flow rate of the outlet stream ($q_1 = q_2$) and, therefore, $(dV/dt) = 0$. Moreover, we know that there will be no generation of chemical species ($G = g_i = 0$). Therefore, in this case, although we do not know the density of the salt solution to convert the volumetric flow rate to mass flow rate, we can consider the salt component



balance with volumetric units because we will continue to work with mass units.

Salt balance (g salt):

$$q_2 \cdot c_2 - q_1 \cdot c_1 + \frac{dV \cdot c}{dt} = 0 \quad \frac{L}{\text{min}} \cdot \frac{g}{L} - \frac{L}{\text{min}} \cdot \frac{g}{L} + \frac{L \cdot g}{\text{min} \cdot L} = 0 \quad \left(\frac{g \text{ salt}}{\text{min}} \right)$$

Since $c_1=0$ is pure water, we eliminate the term for stream 1 in the equation. On the other hand, the salt concentration in stream 2 will be the same as the concentration in the tank at a given time, since the contents of the tank are well agitated ($c_2=c$). Moreover, we are going to solve the differential term in parts and since $dV/dt=0$, the equation is also simplified:

$$q_2 \cdot c + c \cdot \frac{dV}{dt} + V \cdot \frac{dc}{dt} = 0 \quad \Rightarrow \quad q_2 \cdot c + V \cdot \frac{dc}{dt} = 0$$

Rearranging the variables to leave each differential term on one side of the expression, we will have:

$$V \cdot \frac{dc}{dt} = -q_2 \cdot c \quad \Rightarrow \quad \frac{dc}{c} = -\frac{q_2}{V} dt$$

By integrating:

$$\int_{c_0}^c \frac{dc}{c} = -\frac{q_2}{V} \int_0^t dt \quad \Rightarrow \quad \ln c - \ln c_0 = -\frac{q_2}{V} t$$

Therefore, from the theoretical point of view, the mathematical expression that allows us to predict the salt concentration over time in the system under study would be:

$$\ln c = \ln c_0 - \frac{q_2}{V} t$$

*To see if this mathematical model obtained from the application of mass balances is realistic, the best thing to do is to put it to the test. **Do you dare to try it out?***

4.2 Application with experimental data

In order to verify that the theoretical model works, we will validate it with a system similar to the theoretical one of the previous point, but with the numerical data presented in Figure 4. To this end, in the laboratory, we will fill a drum with 15 L of water in which we will place 200 grams of salt; we will submit this to constant agitation that will cause the complete homogenization of the content at all times. The drum will have an aperture in which a conduction will be inserted through which water will enter (stream 1) and it will also have another aperture with another conduction through which solution will be extracted from the interior of the tank (stream 2) with

the same flow as the inlet stream. For this purpose, both pipes will be provided with a throttling valve to open or close them and control the flow of fluids (Figure 5).

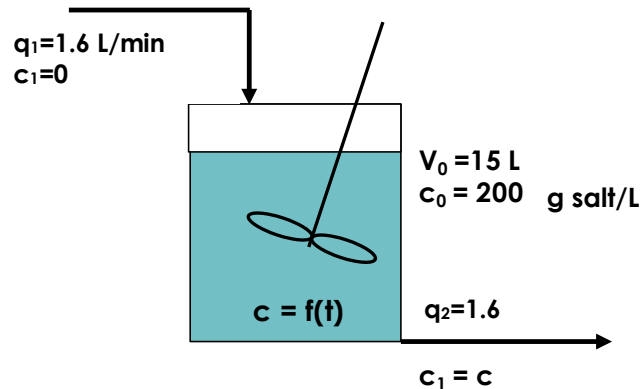


Figure 4. Flow diagram of a tank with a salt solution in which a stream of unsalted water enters and another stream of solution flows out simultaneously and is diluted over time with specific data

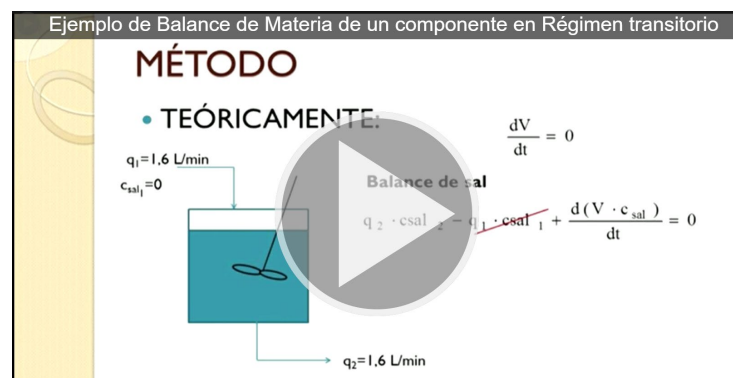


Figure 5. Polimedia (in Spanish) example of the application of mass balances for the prediction of the salt component in a specific process in transient state (Castelló, 2013).

Remember that we want to know how the salt concentration in the tank varies over time. Since the tank is perfectly agitated, that salt concentration will be equal to the salt concentration in the outlet stream. Therefore, once assembled, we will open the two valves of the pipes and collect samples from the outlet stream every two minutes, for approximately 20-30 minutes.

How can we know the salt concentration of the samples we have taken?

Think that salt is an ionic compound and that when dissolved in water, it conducts electricity; so, the higher the concentration of salt in a solution, the greater its conductivity will be. What we will do is measure the conductivity of the samples we have taken. Subsequently, we will have to translate these conductivity measurements into salt content, so we will have to make a **calibration line** that relates the salt concentration to the conductivity. To determine the calibration line, we will prepare solutions of known concentration and measure their conductivity, as

shown in Table 1; we will adjust these data to a line and, thus, we will have an equation that will relate conductivity and salt concentration.

According to the information in Figure 4, we know that the initial concentration of salt in the tank is 13.3 g/L and since the concentration of salt in the tank will decrease, it will be better to draw the calibration line in the range of 0 to 14 g/L because it will be the range of the working salt concentrations. It is important to handle different types of units, so in the practical case the salt concentration is expressed both in mass concentration (g/L) and molar concentration (mol/m³), knowing that the molecular weight of the salt is 58.4 g/mol. Thus, we will be able to predict the salt concentration in the practical case in both units and for this purpose, we will also prepare the calibration lines in both units (Table 1 and Figure 6).

Table 1. Experimental data for the elaboration of the calibration line

Concentration NaCl (g/L)	Concentration NaCl (mol/m ³)	Conductivity (mS/cm)
0,5	8.6	1.42
2	34.2	4.91
4	68.5	8.57
6	102.7	11.64
8	137.0	14.09
10	171.2	16.56
12	205.5	20.60
14	239.7	22.60

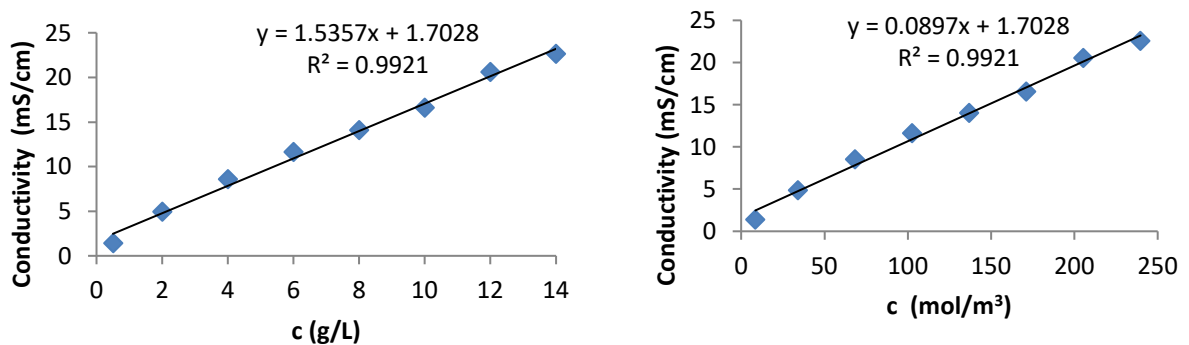


Figure 6. Examples of calibration lines in the working range of the case study

Using the slope and the ordinate at the origin of the linear fits of the calibration lines in Figure 6, we will be able to transform the experimentally measured conductivity values in Table 2 into salt concentrations in the respective units. In addition, in order to arrive at a mathematical expression that allows us to compare it with the theoretical, we will calculate the natural logarithm of the concentration, both in mass and molar units (Table 2).

Table 2. Conductivity values, salt concentration and natural logarithm of this concentration of the samples collected from the experiment at the different times using units of mass or molar concentrations.

t (min)	t (s)	Conductivity (mS/cm)	c_{salt} (g/L)	$\ln c_{\text{salt}}$ (g/L)	c_{salt} (mol/m ³)	$\ln c_{\text{salt}}$ (mol/m ³)
0	0		13.33	2.59	228.31	5.43
2	120	15.73	9.12	2.21	156.14	5.05
4	240	15.39	8.90	2.19	152.38	5.03
6	360	14.04	8.03	2.08	137.44	4.92
8	480	12.79	7.22	1.98	123.62	4.82
10	600	11.26	6.23	1.83	106.69	4.67
12	720	9.80	5.29	1.67	90.54	4.51
14	840	8.49	4.44	1.49	76.04	4.33
16	960	7.37	3.72	1.31	63.65	4.15
18	1080	6.32	3.04	1.11	51.94	3.95
20	1200	5.55	2.54	0.93	43.44	3.77

Next, we will plot the natural logarithm column of the salt concentration versus time and fit the points to a linear equation (Figure 7). The ordinate at the origin will correspond to the value of the natural logarithm of the initial salt concentration in the tank ($\ln c_0$), while the slope of the line will be the numerical value of the quotient between the outlet volumetric flow rate (q_2) and the initial volume of solution in the tank ($V = V_0$).

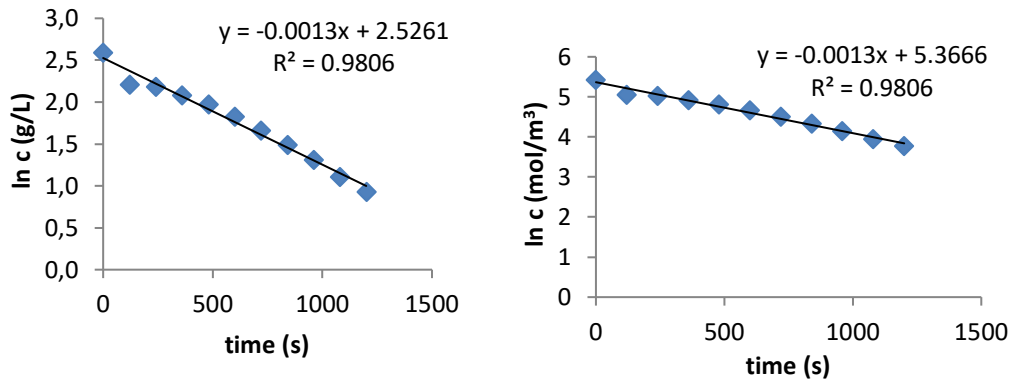


Figure 7. Examples of representation of the natural logarithm values of the salt concentration expressed in mass units or molar units versus time of the experiment

As can be seen, the slope of the linear fits of the graphs in Figure 7 are equal, since in the modeling they are equivalent to the quotient between the outlet flow rate and the initial volume of solution in the tank (q_2/V_0) and these variables are not affected by the way the salt concentration is expressed.



4.3 Comparison of experimental and theoretical parameters

Finally, Table 3 compares the results that would be obtained with the theoretical model ($lnc = lnc_0 - \frac{q_2}{V} t$), replacing the theoretical variables with the experimental data. In this case, we know that $q_2 = 1.6$ mL/min, $c_{salt0} = 13.3$ g/L and the $V_0 = 15$ L.

Table 3. Comparison of the parameters obtained in the adjustment of the experimental data and those resulting from the application of the balances (theoretical model).

Parameters	Theoretical	Experimental
Ordinate at origin (lnc_{salt0}) when c_{salt} (g/L)	2.59	2.53
Ordinate at origin (lnc_{salt0}) when c_{salt} (mol/m ³)	5.43	5.37
Slope (q_2/V_0) when time is in s	0.0018	0.0013

However, the experimental value of the ordinate at the origin is somewhat lower than the experimental. This means that the initial salt concentration was slightly lower than the tank should theoretically have, i.e., less than 13.3 g/L. The same is true for the slope. **Why do you think this might be?**

It could be because the outlet flow rate is lower than it should theoretically be. Another possible reason could be that the initial volume (V_0) is greater than the expected 15 L. Perhaps, both possibilities occur simultaneously or there are other types of mismatches in the experimental values.

In any case, the theoretical and experimental values are practically the same. Therefore, we can conclude that if we know how to correctly formulate and solve the equations of the total and one-component stationary mass balances, we can predict how the concentration varies over time, thus saving us all the experimental setup and data collection.

5 Closing Statement

Throughout this learning object we have seen how to work with the equation of mass balances applied to the salt component in the specific example of a process. In this case, we have dealt with a situation in which the term of accumulation has to be considered because the time variable affects the properties of the system. Furthermore, we have found that the modeling fits the experimentally obtained values very well, corroborating the usefulness of the balances for predicting the variation in the concentration of a component over time. Now you are READY to apply this calculation tool to other common industrial cases.



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