# *Chemical equation balancing*

Chemical equations are a symbolic representation of a chemical reaction. On the left-hand side of an chemical equation is the reactants and the products are on the right-hand side. According to the law of conservation of mass, the mass of the products in a chemical reaction must equal to the mass of the reactants.

Knowing this, if we want to balance a chemical equation we simply add more mass on the side of the equation that has less mass until we bring the system into a state where there is the same mass on both sides. The branch of chemical mathematics called Stoichiometry deals with the weight relations determined by chemical equations and formulas.

Reactions can be feasible and unfeasible. Feasible reactions end up with a consistent equation and have a non-trivial solution, while unfeasible reactions only have solutions that are trivial (all multipliers are zeros).

MatDeck comes implemented with several functions that can help you determine if a chemical equation is feasible or not, and help you find the balanced equation solution if a reaction is feasible.

We will explain the process of balancing a chemical equation implemented in MatDeck on a reaction for photosynthesis. The unbalanced reaction looks like this

$$CO_2 + H_2O = C_6H_{12}O_6 + O_2$$
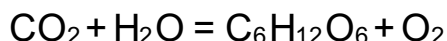
carbon dioxide + water yields glucose + oxygen

Let's insert the unknown coefficients and define them as x_i. The coefficients that we have to determine are all integers.

$$x_1 \cdot CO_2 + x_2 \cdot H_2O = x_3 \cdot C_6H_{12}O_6 + x_4 \cdot O_2$$
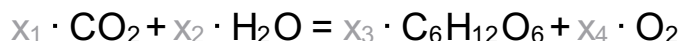
This equation can be formulated as a matrix equation. Let there be **n** distinct elements and **m** distinct reactants as well as reaction products. We will form a n x m matrix known as **A**, called the reaction matrix, whose (i , j) th element a_{ij} is the number of atoms of type *i* in each reactant or product. Matrix elements can be positive or negative based on their position in the equation, coefficients that correspond to a reactant are positive and coefficients that correspond to a product are negative. This way we have a homogeneous matrix equation

$$A_{mat} \cdot x = 0$$

Where x is the column vector of unknown coefficients and 0 is the null column vector.
To calculate the coefficients of matrix A, we use the function ***chem reactm()*** whose arguments are left-hand and right-hand side of starting the chemical reaction.

$$A_{mat} := chem\ reactm\left(CO_2 + H_2O \ , \ C_6H_{12}O_6 + O_2\right)$$

$$A_{mat} = \begin{bmatrix} 1 & 0 & -6 & 0 \\ 2 & 1 & -6 & -2 \\ 0 & 2 & -12 & 0 \end{bmatrix}$$

In this matrix, every column presents one chemical compound and every row presents the number of atoms of a chemical element in that compound.

$$\begin{bmatrix} . & CO_2 & H_2O & C_6H_{12}O_6 & O_2 \\ C & 1 & 0 & -6 & 0 \\ O & 2 & 1 & -6 & -2 \\ H & 0 & 2 & -12 & 0 \end{bmatrix}$$

There is a function that can the return number of atoms of each chemical element in the compound that we insert. The name of this function is **chem parse()** and it can help you to determine which row of the coefficient matrix presents the number of atoms for a specific chemical element. For example, if we insert $C_6H_{12}O_6$ as an argument we will have

$$\text{chem parse}(C_6H_{12}O_6) = \begin{bmatrix} \begin{bmatrix} 6 \\ 12 \\ 6 \end{bmatrix} & \begin{bmatrix} C \\ H \\ O \end{bmatrix} \end{bmatrix}$$

As you can see, this is the third row of coefficients matrix that represents the number of atoms for each compound element. The convention we have used is that the elements are taken in the order in which they occur in equation.

The solution of a homogeneous equation, $Ax = 0$, where A is $n \times m$ matrix of rank r is $x = Pz$. Rank of matrix P is k. The different cases that are possible depend on the following conditions:

$n \geq m = r$, $k = m - r = 0$	Reaction is infeasible
$n \geq m, r = m - 1, k = m - r = 1$	Reaction is feasible with unique solution
$n \geq m, r < m - 1, k = m - r > 1$	Reaction is feasible with nonunique solution
$n < m, r \leq n, k = m - r \geq 1$	Reaction is feasible with nonunique solution if $k > 1$

To calculate the multiplication of coefficients use the function **chem coeff()**

$$\text{chem coeff}\left(\begin{bmatrix} 1 & 0 & -6 & 0 \\ 2 & 1 & -6 & -2 \\ 0 & 2 & -12 & 0 \end{bmatrix} \right) = \begin{bmatrix} 6 & 6 & 1 & 6 \end{bmatrix}$$

The argument of this function is the coefficient matrix of the starting equation, while the result vector contains chemical compounds multipliers.

There is an easy way to balance the equation. The procedure is

1) $CO_2 + H_2O = C_6H_{12}O_6 + O_2$
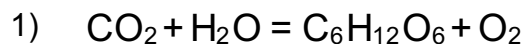
> Create the equation that you want to be balanced
> Use Ctrl. + = key combination to create an equal sign

2) $6\ CO_2 + 6\ H_2O \rightarrow C_6H_{12}O_6 + 6\ O_2$
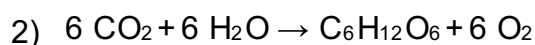
> Position the mouse cursor above the equal sign and press the right mouse button
> Equal sign will transform to dart and equation will be balanced (if reaction is feasible)

If you press the right mouse button again while the mouse cursor is above the dart, it will transform it into two darts. The equation will remain balanced, this is only a visual change.

$$6\ CO_2 + 6\ H_2O \leftrightharpoons C_6H_{12}O_6 + 6\ O_2$$
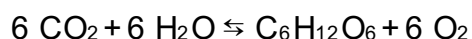
At the end, we have balanced the inserted equation in the process that is simple and efficient. You can use the functions that we have described in this document to help you in the process of balancing equations.