

Balancing Chemical Equations using Matrices

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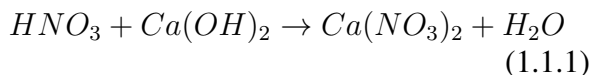
Abstract—This manual shows how to balance chemical equations using matrices. based on exercise from the NCERT textbooks from Class 6-12.

Download python codes using

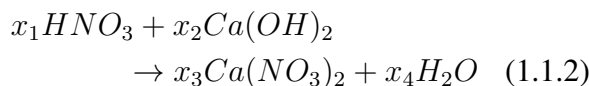
svn co <https://github.com/gadepall/school/trunk/ncert/computation/codes>

1 EXAMPLES

1.1. Balance the following chemical equation.



Solution: Let the balanced version of (1.1.1) be



which results in the following equations:

$$(x_1 + 2x_2 - 2x_4)H = 0 \quad (1.1.3)$$

$$(x_1 - 2x_3)N = 0 \quad (1.1.4)$$

$$(3x_1 + 2x_2 - 6x_3 - x_4)O = 0 \quad (1.1.5)$$

$$(x_2 - x_3)Ca = 0 \quad (1.1.6)$$

which can be expressed as

$$x_1 + 2x_2 + 0x_3 - 2x_4 = 0 \quad (1.1.7)$$

$$x_1 + 0x_2 - 2x_3 + 0x_4 = 0 \quad (1.1.8)$$

$$3x_1 + 2x_2 - 6x_3 - x_4 = 0 \quad (1.1.9)$$

$$0x_1 + x_2 - x_3 + 0x_4 = 0 \quad (1.1.10)$$

resulting in the matrix equation

$$\begin{pmatrix} 1 & 2 & 0 & -2 \\ 1 & 0 & -2 & 0 \\ 3 & 2 & -6 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \mathbf{x} = \mathbf{0} \quad (1.1.11)$$

where,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \quad (1.1.12)$$

(1.1.11) can be reduced as follows

$$\begin{pmatrix} 1 & 2 & 0 & -2 \\ 1 & 0 & -2 & 0 \\ 3 & 2 & -6 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \quad (1.1.13)$$

$$\begin{matrix} \xleftarrow{R_2 \leftarrow R_2 - R_1} \\ \xleftarrow{R_3 \leftarrow \frac{R_3}{3} - R_1} \end{matrix} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & -2 & -2 & 2 \\ 0 & -\frac{4}{3} & -2 & \frac{5}{3} \\ 0 & 1 & -1 & 0 \end{pmatrix} \quad (1.1.14)$$

$$\xleftarrow{R_2 \leftarrow -\frac{R_2}{2}} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & 1 & 1 & -1 \\ 0 & -\frac{4}{3} & -2 & \frac{5}{3} \\ 0 & 1 & -1 & 0 \end{pmatrix} \quad (1.1.15)$$

$$\begin{matrix} \xleftarrow{R_3 \leftarrow R_3 + \frac{4}{3}R_2} \\ \xleftarrow{R_4 \leftarrow R_4 - R_2} \end{matrix} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & -\frac{2}{3} & \frac{1}{3} \\ 0 & 0 & -2 & 1 \end{pmatrix} \quad (1.1.16)$$

$$\begin{matrix} \xleftarrow{R_1 \leftarrow R_1 - 2R_2} \\ \xleftarrow{R_3 \leftarrow -\frac{3}{2}R_3} \end{matrix} \begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & -2 & 1 \end{pmatrix} \quad (1.1.17)$$

$$\xleftarrow{R_4 \leftarrow R_4 + 2R_3} \begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (1.1.18)$$

$$\begin{matrix} \xleftarrow{R_1 \leftarrow R_1 + 2R_3} \\ \xleftarrow{R_2 \leftarrow R_2 - R_3} \end{matrix} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (1.1.19)$$

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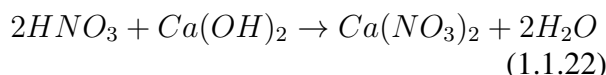
Thus,

$$x_1 = x_4, x_2 = \frac{1}{2}x_4, x_3 = \frac{1}{2}x_4 \quad (1.1.20)$$

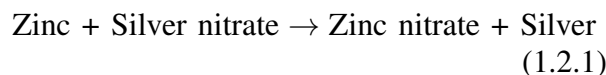
$$\Rightarrow \mathbf{x} = x_4 \begin{pmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 1 \\ 2 \end{pmatrix} \quad (1.1.21)$$

by substituting $x_4 = 2$

Hence, (1.1.2) finally becomes

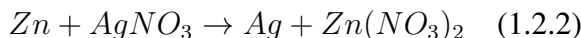


1.2. Balance the following chemical equation.

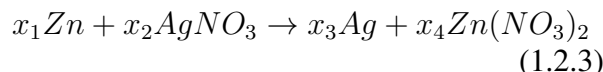


Solution:

1.2.1 can be written as



Suppose the balanced form of the equation is



which results in the following equations:

$$(x_1 - 2x_4)Zn = 0 \quad (1.2.4)$$

$$(x_2 - x_3)Ag = 0 \quad (1.2.5)$$

$$(x_3 - 2x_4)N = 0 \quad (1.2.6)$$

$$(3x_3 - 6x_4)O = 0 \quad (1.2.7)$$

which can be expressed as

$$x_1 + 0x_2 + 0x_3 - x_4 = 0 \quad (1.2.8)$$

$$0x_1 + x_2 - x_3 + 0x_4 = 0 \quad (1.2.9)$$

$$0x_1 + 0x_2 + x_3 - 2x_4 = 0 \quad (1.2.10)$$

$$0x_1 + 0x_2 + 3x_3 - 6x_4 = 0 \quad (1.2.11)$$

resulting in the matrix equation

$$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 3 & -6 \end{pmatrix} \mathbf{x} = \mathbf{0} \quad (1.2.12)$$

where,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \quad (1.2.13)$$

(1.2.12) can be reduced as

$$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 3 & -6 \end{pmatrix} \xrightarrow{R_4 \leftarrow R_4 - 3R_3} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (1.2.14)$$

Thus,

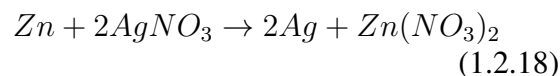
$$x_1 = x_4, x_2 = 2x_4, x_3 = 2x_4 \quad (1.2.15)$$

$$\Rightarrow \mathbf{x} = \begin{pmatrix} x_4 \\ 2x_4 \\ 2x_4 \\ x_4 \end{pmatrix} = x_4 \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \end{pmatrix} \quad (1.2.16)$$

by substituting $x_4 = 1$, we get

$$\Rightarrow \mathbf{x} = \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \end{pmatrix} \quad (1.2.17)$$

Hence, (1.2.3) finally becomes

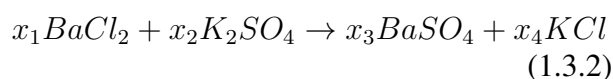


1.3. Write the balanced chemical equations for the following reaction :



Solution: We know that the number of atoms of each element remains the same, before and after a chemical reaction.

Equation (1.3.1) can be written as



Element wise contribution in forming the respective chemical compound can be written in the form of equation as

$$Ba : x_1 + 0x_2 - x_3 - 0x_4 = 0 \quad (1.3.3)$$

$$Cl : 2x_1 + 0x_2 - 0x_3 - 1x_4 = 0 \quad (1.3.4)$$

$$K : 0x_1 + 2x_2 - 0x_3 - 1x_4 = 0 \quad (1.3.5)$$

$$S : 0x_1 + 1x_2 - 1x_3 - 0x_4 = 0 \quad (1.3.6)$$

$$O : 0x_1 + 4x_2 - 4x_3 - 0x_4 = 0 \quad (1.3.7)$$

In matrix form this can be written as

$$A\mathbf{x} = 0 \quad (1.3.8)$$

$$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 2 & 0 & 0 & -1 \\ 0 & 2 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 4 & -4 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (1.3.9)$$

Using Gaussian Elimination method

$$\xleftrightarrow{R_2 \leftrightarrow R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & | & 0 \\ 0 & 4 & -4 & 0 & | & 0 \\ 0 & 2 & 0 & -1 & | & 0 \\ 0 & 1 & -1 & 0 & | & 0 \\ 2 & 0 & 0 & -1 & | & 0 \end{pmatrix} \quad (1.3.10)$$

$$\xleftrightarrow{R_5 \leftarrow 2R_1 - R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & | & 0 \\ 0 & 4 & -4 & 0 & | & 0 \\ 0 & 2 & 0 & -1 & | & 0 \\ 0 & 1 & -1 & 0 & | & 0 \\ 0 & 0 & -2 & 1 & | & 0 \end{pmatrix} \quad (1.3.11)$$

$$\xleftrightarrow{\begin{matrix} R_3 \leftarrow 2R_3 - R_2 \\ R_4 \leftarrow 4R_4 - R_2 \end{matrix}} \begin{pmatrix} 1 & 0 & -1 & 0 & | & 0 \\ 0 & 4 & -4 & 0 & | & 0 \\ 0 & 0 & 4 & -2 & | & 0 \\ 0 & 0 & 0 & 0 & | & 0 \\ 0 & 0 & -2 & 1 & | & 0 \end{pmatrix} \quad (1.3.12)$$

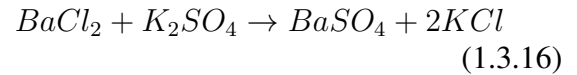
$$\xleftrightarrow{R_5 \leftrightarrow R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & | & 0 \\ 0 & 4 & -4 & 0 & | & 0 \\ 0 & 0 & 4 & -2 & | & 0 \\ 0 & 0 & -2 & 1 & | & 0 \\ 0 & 0 & 0 & 0 & | & 0 \end{pmatrix} \quad (1.3.13)$$

$$\xleftrightarrow{R_4 \leftarrow 2R_4 - R_3} \begin{pmatrix} 1 & 0 & -1 & 0 & | & 0 \\ 0 & 4 & -4 & 0 & | & 0 \\ 0 & 0 & 4 & -2 & | & 0 \\ 0 & 0 & 0 & 0 & | & 0 \\ 0 & 0 & 0 & 0 & | & 0 \end{pmatrix} \quad (1.3.14)$$

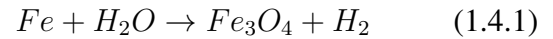
Clearly the system is linearly dependent. Therefore by fixing the value of $x_4 = 2$, one of the possible vectors \mathbf{x} is

$$\mathbf{x} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 2 \end{pmatrix} \quad (1.3.15)$$

Hence by putting the values of x_1, x_2, x_3, x_4 in equation (1.3.1) we get our balanced chemical equation as

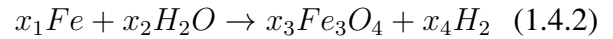


1.4. Balance the following chemical equation.



Solution:

Let the balanced version of (1.4.1) be



which results in the following equations

$$\begin{aligned} (x_1 - 3x_3) Fe &= 0 \\ (2x_2 - 2x_4) H &= 0 \\ (x_2 - 4x_3) O &= 0 \end{aligned} \quad (1.4.3)$$

which can be expressed as

$$\begin{aligned} x_1 + 0.x_2 - 3x_3 + 0.x_4 &= 0 \\ 0.x_1 + 2x_2 + 0.x_3 - 2x_4 &= 0 \\ 0.x_1 + x_2 - 4x_3 + 0.x_4 &= 0 \end{aligned} \quad (1.4.4)$$

resulting in the matrix equation

$$\begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 2 & 0 & -2 \\ 0 & 1 & -4 & 0 \end{pmatrix} \mathbf{x} = \mathbf{0} \quad (1.4.5)$$

where

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \quad (1.4.6)$$

(1.4.5) can be row reduced as follows

$$\begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 2 & 0 & -2 \\ 0 & 1 & -4 & 0 \end{pmatrix} \xleftrightarrow{R_2 \leftarrow \frac{R_2}{2}} \begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 1 & -4 & 0 \end{pmatrix} \quad (1.4.7)$$

$$\xleftrightarrow{R_3 \leftarrow R_3 - R_2} \begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -4 & 1 \end{pmatrix} \quad (1.4.8)$$

$$\xleftrightarrow{R_1 \leftarrow 4R_1 - 3R_3} \begin{pmatrix} 4 & 0 & 0 & -3 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -4 & 1 \end{pmatrix} \quad (1.4.9)$$

$$\xleftrightarrow{\begin{matrix} R_1 \leftarrow \frac{1}{4} \\ R_3 \leftarrow -\frac{1}{4}R_3 \end{matrix}} \begin{pmatrix} 1 & 0 & 0 & -\frac{3}{4} \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -\frac{1}{4} \end{pmatrix} \quad (1.4.10)$$

Thus,

$$x_1 = \frac{3}{4}x_4, x_2 = x_4, x_3 = \frac{1}{4}x_4 \quad (1.4.11)$$

$$(1.4.12)$$

$$\Rightarrow \mathbf{x} = x_4 \begin{pmatrix} \frac{3}{4} \\ 1 \\ \frac{1}{4} \\ 1 \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 1 \\ 4 \end{pmatrix} \quad (1.4.13)$$

upon substituting $x_4 = 4$. (1.4.2) then becomes

