Balancing Chemical Equations using Matrices

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Contents

***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

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svn co https://github.com/gadepall/school/trunk/
    ncert/computation/codes
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1 Examples

1.1. Balance the following chemical equation.

$$HNO_3 + Ca(OH)_2 \to Ca(NO_3)_2 + H_2O \tag{1.1.1}$$

Solution: Let the balanced version of (1.1.1) be

$$x_1HNO_3 + x_2Ca(OH)_2 \to x_3Ca(NO_3)_2 + x_4H_2O \tag{1.1.2}$$

which results in the following equations:

$$(x_1 + 2x_2 - 2x_4)H = 0 \tag{1.1.3}$$
$$(x_1 - 2x_3)N = 0 \tag{1.1.4}$$
$$(3x_1 + 2x_2 - 6x_3 - x_4)O = 0 \tag{1.1.5}$$
$$(x_2 - x_3)Ca = 0 \tag{1.1.6}$$

which can be expressed as

$$x_1 + 2x_2 + 0x_3 - 2x_4 = 0 \tag{1.1.7}$$
$$x_1 + 0x_2 - 2x_3 + 0.x_4 = 0 \tag{1.1.8}$$
$$3x_1 + 2x_2 - 6x_3 - x_4 = 0 \tag{1.1.9}$$
$$0x_1 + x_2 - x_3 + 0.x_4 = 0 \tag{1.1.10}$$

resulting in the matrix equation

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

where,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \tag{1.1.12}$$

(1.1.11) can be reduced as follows

$$\begin{pmatrix} 1 & 2 & 0 & -2 \\ 1 & 0 & -2 & 0 \\ 3 & 2 & -6 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \tag{1.1.13}$$

$$\xleftrightarrow[R_3 \leftarrow \frac{R_3}{3} - R_1]{R_2 \leftarrow R_2 - R_1} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & -2 & -2 & 2 \\ 0 & -\frac{4}{3} & -2 & \frac{5}{3} \\ 0 & 1 & -1 & 0 \end{pmatrix} \tag{1.1.14}$$

$$\xleftrightarrow{R_2 \leftarrow -\frac{R_2}{2}} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & 1 & 1 & -1 \\ 0 & -\frac{4}{3} & -2 & \frac{5}{3} \\ 0 & 1 & -1 & 0 \end{pmatrix} \tag{1.1.15}$$

$$\xleftrightarrow[R_4 \leftarrow R_4 - R_2]{R_3 \leftarrow R_3 + \frac{4}{3}R_2} \begin{pmatrix} 1 & 2 & 0 & -2 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & -\frac{2}{3} & \frac{1}{3} \\ 0 & 0 & -2 & 1 \end{pmatrix} \tag{1.1.16}$$

$$\xleftrightarrow[R_3 \leftarrow -\frac{3}{2}R_3]{R_1 \leftarrow R_1 - 2R_2} \begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & -2 & 1 \end{pmatrix} \tag{1.1.17}$$

$$\xleftrightarrow{R_4 \leftarrow R_4 + 2R_3} \begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{1.1.18}$$

$$\xleftrightarrow[R_2 \leftarrow R_2 - R_3]{R_1 \leftarrow R_1 + 2R_3} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{1.1.19}$$

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Thus,

$$x_1 = x_4, x_2 = \frac{1}{2}x_4, x_3 = \frac{1}{2}x_4 \tag{1.1.20}$$

$$\implies \quad \mathbf{x} = x_4 \begin{pmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 1 \\ 2 \end{pmatrix} \tag{1.1.21}$$

by substituting $x_4 = 2$

Hence, (1.1.2) finally becomes

$$2HNO_3 + Ca(OH)_2 \rightarrow Ca(NO_3)_2 + 2H_2O \tag{1.1.22}$$

1.2. Balance the following chemical equation.

$$\text{Zinc + Silver nitrate} \rightarrow \text{Zinc nitrate + Silver} \tag{1.2.1}$$

Solution:
1.2.1 can be written as

$$Zn + AgNO_3 \rightarrow Ag + Zn(NO_3)_2 \tag{1.2.2}$$

Suppose the balanced form of the equation is

$$x_1 Zn + x_2 AgNO_3 \rightarrow x_3 Ag + x_4 Zn(NO_3)_2 \tag{1.2.3}$$

which results in the following equations:

$$(x_1 - 2x_4)Zn = 0 \tag{1.2.4}$$
$$(x_2 - x_3)Ag = 0 \tag{1.2.5}$$
$$(x_3 - 2x_4)N = 0 \tag{1.2.6}$$
$$(3x_3 - 6x_4)O = 0 \tag{1.2.7}$$

which can be expressed as

$$x_1 + 0x_2 + 0x_3 - x_4 = 0 \tag{1.2.8}$$
$$0x_1 + x_2 - x_3 + 0x_4 = 0 \tag{1.2.9}$$
$$0x_1 + 0x_2 + x_3 - 2x_4 = 0 \tag{1.2.10}$$
$$0x_1 + 0x_2 + 3x_3 - 6x_4 = 0 \tag{1.2.11}$$

resulting in the matrix equation

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

where,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \tag{1.2.13}$$

(1.2.12) can be reduced as

$$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 3 & -6 \end{pmatrix}$$
$$\xleftrightarrow{R_4 \leftarrow R_4 - 3R_3} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{1.2.14}$$

Thus,

$$x_1 = x_4, x_2 = 2x_4, x_3 = 2x_4 \tag{1.2.15}$$

$$\implies \quad \mathbf{x} = \begin{pmatrix} x_4 \\ 2x_4 \\ 2x_4 \\ x_4 \end{pmatrix} = x_4 \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \end{pmatrix} \tag{1.2.16}$$

by substituting $x_4 = 1$, we get

$$\implies \quad \mathbf{x} = \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \end{pmatrix} \tag{1.2.17}$$

Hence, (1.2.3) finally becomes

$$Zn + 2AgNO_3 \rightarrow 2Ag + Zn(NO_3)_2 \tag{1.2.18}$$

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

$$BaCl_2 + K_2SO_4 \rightarrow BaSO_4 + KCl \tag{1.3.1}$$

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

$$x_1 BaCl_2 + x_2 K_2SO_4 \rightarrow x_3 BaSO_4 + x_4 KCl \tag{1.3.2}$$

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

$$\xleftrightarrow{R_2 \leftrightarrow R_5} \left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 4 & -4 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 2 & 0 & 0 & -1 & 0 \end{array}\right) \quad (1.3.10)$$

$$\xleftrightarrow{R_5 \leftarrow 2R_1 - R_5} \left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 4 & -4 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 \end{array}\right) \quad (1.3.11)$$

$$\xleftrightarrow[R_4 \leftarrow 4R_4 - R_2]{R_3 \leftarrow 2R_3 - R_2} \left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 4 & -4 & 0 & 0 \\ 0 & 0 & 4 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 \end{array}\right) \quad (1.3.12)$$

$$\xleftrightarrow{R_5 \leftrightarrow R_5} \left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 4 & -4 & 0 & 0 \\ 0 & 0 & 4 & -2 & 0 \\ 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right) \quad (1.3.13)$$

$$\xleftrightarrow{R_4 \leftarrow 2R_4 - R_3} \left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 4 & -4 & 0 & 0 \\ 0 & 0 & 4 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right) \quad (1.3.14)$$

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

$$BaCl_2 + K_2SO_4 \rightarrow BaSO_4 + 2KCl \quad (1.3.16)$$

1.4. Balance the following chemical equation.

$$Fe + H_2O \rightarrow Fe_3O_4 + H_2 \quad (1.4.1)$$

Solution:
Let the balanced version of (1.4.1) be

$$x_1Fe + x_2H_2O \rightarrow x_3Fe_3O_4 + x_4H_2 \quad (1.4.2)$$

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

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

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

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

$$\xleftrightarrow[R_3 \leftarrow -\frac{1}{4}R_3]{R_1 \leftarrow \frac{1}{4}} \begin{pmatrix}1 & 0 & 0 & -\frac{3}{4}\\ 0 & 1 & 0 & -1\\ 0 & 0 & 1 & -\frac{1}{4}\end{pmatrix} \tag{1.4.10}$$

Thus,

$$x_1 = \frac{3}{4}x_4, x_2 = x_4, x_3 = \frac{1}{4}x_4 \tag{1.4.11}$$

$$\tag{1.4.12}$$

$$\implies \mathbf{x} = x_4 \begin{pmatrix}\frac{3}{4}\\ 1\\ \frac{1}{4}\\ 1\end{pmatrix} = \begin{pmatrix}3\\ 4\\ 1\\ 4\end{pmatrix} \tag{1.4.13}$$

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

$$3Fe + 4H_2O \to Fe_3O_4 + 4H_2 \tag{1.4.14}$$