

Optimization through School Geometry



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Abstract—This manual shows how to balance chemical equations using matrices.

Download python codes using

svn co https://github.com/gadepall/school/trunk/ training

Balance the following chemical equation

$$Fe + H_2O \rightarrow Fe_3O_4 + H_2 \tag{1}$$

Solution: Let the balanced version of (1) be

$$x_1Fe + x_2H_2O \rightarrow x_3Fe_3O_4 + x_4H_2$$
 (2)

which results in the following equations

$$(x_1 - 3x_3) Fe = 0$$

$$(2x_2 - 2x_4) H = 0$$

$$(x_2 - 4x_3) H = 0$$

$$x_1 + 0.x_2 - 3x_3 + 0.x_4 = 0$$

$$\implies 0.x_1 + 2x_2 + 0.x_3 - 2x_4 = 0$$
(4)

$$\implies 0.x_1 + 2x_2 + 0.x_3 - 2x_4 = 0$$

$$0.x_1 + x_2 - 4x_3 + 0.x_4 = 0$$

resulting in the matrix equation

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

where

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \tag{6}$$

The matrix in (5) can be row reduced as follows

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

$$(7)$$

$$\xrightarrow{R_3 \leftarrow R_3 - R_2}
\begin{pmatrix}
1 & 0 & -3 & 0 \\
0 & 1 & 0 & -1 \\
0 & 0 & -4 & 1
\end{pmatrix}
\xrightarrow{R_1 \leftarrow 4R_1 - 3R_3}
\begin{pmatrix}
4 & 0 & 0 & -3 \\
0 & 1 & 0 & -1 \\
0 & 0 & -4 & 1
\end{pmatrix}$$

$$(8)$$

$$\xrightarrow[R_3 \leftarrow -\frac{1}{4}R_3]{1 \quad 0 \quad 0 \quad -\frac{3}{4} \\ 0 \quad 1 \quad 0 \quad -1 \\ 0 \quad 0 \quad 1 \quad -\frac{1}{4}}$$

$$(9)$$

Thus,

$$\mathbf{x} = x_4 \begin{pmatrix} \frac{3}{4} \\ 1 \\ \frac{1}{4} \\ 1 \end{pmatrix} \tag{10}$$

Substituting $x_4 = 4$ in (10),

$$\mathbf{x} = \begin{pmatrix} 3 \\ 4 \\ 1 \\ 4 \end{pmatrix} \tag{11}$$

(5) and (2) becomes

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$$
 (12)

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