

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/chemistry/codes

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) Thus,

which results in the following equations

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

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

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

$$x_1 - 3x_3 = 0$$

$$\Rightarrow 2x_2 - 2x_4 = 0$$

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

resulting in the matrix equation

$$\begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 2 & 0 & -2 \\ 0 & 1 & -4 & 0 \end{pmatrix} \mathbf{x} = \mathbf{0}$$
 (5)

where

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

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The matrix in (6) can be row reduced as follows

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

$$(1 \quad 0 \quad 3 \quad 0) \qquad (4 \quad 0 \quad 0 \quad 3)$$

$$\stackrel{R_3 \leftarrow R_3 - R_2}{\longleftrightarrow} \begin{pmatrix} 1 & 0 & -3 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -4 & 1 \end{pmatrix} \stackrel{R_1 \leftarrow 4R_1 - 3R_3}{\longleftrightarrow} \begin{pmatrix} -4 & 0 & 0 & -3 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -4 & 1 \end{pmatrix} \tag{8}$$

$$\xrightarrow[R_3 \leftarrow -\frac{1}{4}R_3]{1} \begin{pmatrix} 1 & 0 & 0 & \frac{3}{4} \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & \frac{1}{4} \end{pmatrix}$$

$$(9)$$

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