Nomenclature

Latin letters

a_i	activity of species i
a_{ki}	subscript to element k in molecular formula of species i
$\mathbf{A}$	formula matrix: the $(M \times N)$ matrix whose entries are a_{ki}
$\mathbf{A}^*$	unit matrix or row-reduced echelon form of $\mathbf{A}$
b_k	number of moles of element k
$\mathbf{b}$	element-abundance vector with entries b_k
C	number of component species; number of linearly independent atom-balance equations
CRS	chemical reaction stoichiometry
F	number of degrees of freedom
F_s	number of stoichiometric degrees of freedom
G	Gibbs function
ΔG_j	change in Gibbs function for chemical equation j
ΔG_j^0	standard change in Gibbs function for chemical equation j
K_{aj}	equilibrium constant for chemical equation j
K_w	equilibrium constant for water dissociation
M	number of elements
MRM	matrix reduction method
$\mathbf{n}$	species-abundance vector with entries n_i
n_i	number of moles of species i
δn_i	change in number of moles of species i
$\boldsymbol{\delta}\mathbf{n}$	species-abundance-change vector with entries δn_i
N	number of species
$\mathbf{N}$	stoichiometric matrix with elements ν_{ij}
$\mathbf{N}^*$	reduced stoichiometric matrix obtained from the matrix $\mathbf{N}$
p	(protonic) charge
P	pressure
P^0	standard-state pressure
r	number of stoichiometric restrictions
R	maximum or proper number of linearly independent chemical equations
T	temperature (absolute)
X^0	standard-state composition

Greek letters

μ_i	chemical potential of species i

$\mu_i^0(T, P^0, X^0)$	standard chemical potential of species i at the system T, the standard-state pressure P^0, and the standard-state composition X^0
$\mu_i^0(T)$	standard chemical potential of species i at the system T (arguments P^0, X^0 are suppressed)
ν_i	stoichiometric coefficient of species i in a single chemical equation
ν_{ij}	stoichiometric coefficient of species i in chemical equation j
$\boldsymbol{\nu}$	stoichiometric vector with entries ν_i in a single chemical equation

Subscripts

i, j, k	dummy indices

Other symbols

$=$	denotes chemical equation
$\rightarrow$	denotes irreversible chemical reaction
$\rightleftharpoons$	denotes reaction at equilibrium
T	as superscript, denotes transpose of a vector

Literature Cited

[1] Anderson, G. M., and D. A. Crerar. *Thermodynamics in Geochemistry.* Oxford U. Press, Oxford, 1993.

[2] Apse, J. I., and R. W. Missen. "Natural Equilibrium Distribution of Methane and the Deuteromethanes". *J. Chem. Educ.*, **44**:30, 1967.

[3] Betz, M.L., J. P. Hupke, and D. W. Dickerhoof. "ChemBalance Wizard". *http://www.mines.edu/academic/chemistry/chembal/*, 1997.

[4] Björnbom, P. H. *Ind. Eng. Chem., Fundam.*, **14**:102, 1975.

[5] Björnbom, P. H. "letter to the editor concerning 'Some Remarks on the Calculation of Complex Chemical Equilibria by General Methods' by Smith". *Ind. Eng. Chem., Fundam.*, **17**:69, 1978.

[6] Bottomley, J. "Note on a Method for Determining the Coefficients in Chemical Equations". *J. Chem. News J. Phys. Sci.*, **37**:110–111, 1878.

[7] Brown, J,P., L. P. Brown, and R. M. Redd. "A Computer Program for Balancing Chemical Equations". *J. Chem. Educ.*, **49**:754, 1972.

[8] Campanario, J. M. "Automatic 'Balancing' of Chemical Equations". *Computers Chem.*, **19**:85–90, 1995.

[9] Carrano, S. A. "Balancing an Atypical Redox Equation". *J. Chem. Educ.*, **55**:382, 1978.

[10] Cheluget, E. L., R. W. Missen, and W. R. Smith. "Computer Calculation of Ionic Equilibria Using Species- or Reaction-Related Thermodynamic Data". *J. Phys. Chem.*, **91**:2428–2432, 1987.

[11] Cobranchi, D.P., and E. M. Eyring. "Calculating Equilibrium Concentrations by the Continuation Method". *J. Chem. Educ.*, **68**:40–41, 1991.

[12] Denbigh, K. G. *The Principles of Chemical Equilibrium.* Cambridge U. Press, 4th edition, 1981.

[13] Ferguson, L. A. "How Do I Balance Thee?...Let Me Count the Ways". *J. Chem. Educ.*, **73**:1129, 1996.

[14] Herndon, J. A. "On Balancing Chemical Equations: Past and Present". *J. Chem. Educ.*, **74**:1359–1362, 1997.

[15] Jensen, W. B. "Unbalanced Chemical Equations"(letter to the editor). *J. Chem. Educ.*, **64**:646, 1987.

[16] Kimura, R. T., Haunschild, P. A., and K. C. Lidell. *Metallurgical Trans.*, **15B**:213–219, 1984.

[17] Kubachewski, O., and C. B. Alcock. *Metallurgical Thermochemistry.* Pergamon, New York, 5th edition, 1979.

[18] Laidler, K. J., and M. T. H. Liu. *Proc. Roy. Soc.*, **A297**:365, 1967.

[19] Madeley, W. D., and J. M. Toguri. "The Application of Free Energy Minimization Techniques to Determine Equilibrium Compositions in Systems of Metallurgical Interest". *Can. Metall. Quart.*, **12**:71–78, 1973.

[20] McBride, L. E., and K. L. Adams. "The G. Frederick Smith Chemical Company". *J. Chem. Educ.*, **61**:625–626, 1984.

[21] Missen, R. W. "Balancing Equations"(letter to the editor). *J. Chem. Educ.*, **47**:785, 1970.

[22] Missen, R. W., and W. R. Smith. Letter to the editor concerning Olson(1997). *J. Chem. Educ.*, **75**:286, 1998.

[23] Missen, R.W., and W. R. Smith. "A Question of Basic Chemical Literacy?". *J. Chem. Educ.*, **66**:217–218, 1989. *erratum*, **66**:534.

[24] Missen, R.W., and W. R. Smith. "The Permanganate-Peroxide Reaction: Illustration of a Stoichiometric Restriction". *J. Chem. Educ.*, **67**:876–877, 1990.

[25] Missen, R.W., C. A. Mims, and B. A. Saville. *Introduction to Chemical Reaction Engineering and Kinetics*. Wiley, New York, 1999. in press.

[26] Noble, B. and J. W. Daniel. *Applied Linear Algebra*. Prentice-Hall, Englewood Cliffs, New Jersey, 2nd edition, 1977.

[27] Nordstrom, D. K., and J. L. Munoz. *Geochemical Thermodynamics*. Blackwell Scientific Publications, Cambridge, MA, 2nd edition, 1994.

[28] Olson, J. A. "An Analysis of the Algebraic Method for Balancing Chemical Reactions". *J. Chem. Educ.*, **74**:538–542, 1997.

[29] Porter, S. K. "How Should Equation Balancing Be Taught?". *J. Chem. Educ.*, **62**:507–508, 1985.

[30] Ramette, R. W. "REACT: Exploring Practical Thermodynamic and Equilibrium Calculations". *J. Chem. Educ.: Software*, **8**(B1):13, 1995.

[31] Rice, F. O., and K. F. Herzfeld. *J. Am. Chem. Soc.*, **56**:284, 1934.

[32] Rosen, A. I. "A Computer Program Designed to Balance Inorganic Chemical Reactions". *J. Chem. Educ.*, **54**:704, 1977.

[33] Sanderson, R. V., and H. H. Y. Chien. "Simultaneous Chemical and Phase Equilibrium Calculations". *Ind. Eng. Chem. Proc. Des. Dev.*, **12**:81–85, 1973.

[34] Segraves, R. O., and D. Wickersham. "Learn Lessons from the PEPCON Explosions". *Chem. Eng. Prog.*, **87**:65–69, June 1991.

[35] Smith, W. R. "Some Remarks on the Calculation of Complex Chemical Equilibria by General Methods". *Ind. Eng. Chem., Fundam.*, **15**:227–229, 1976.

[36] Smith, W. R. "reply to letter to the editor by Björnbom concerning 'Some Remarks on the Calculation of Complex Chemical Equilibria by General Methods'". *Ind. Eng. Chem., Fundam.*, **17**:69–70, 1978.

[37] Smith, W. R., and R. W. Missen. "What is Chemical Stoichiometry?". *Chem. Eng. Educ.*, **13**:26–32, 1979.

[38] Smith, W. R., and R. W. Missen. *Chemical Reaction Equilibrium Analysis: Theory and Algorithms*. Wiley-Interscience, New York, 1982. reprinted with corrections, Krieger, Malabar, FL., 1991.

[39] Smith, W. R., and R. W. Missen. "Using Mathematica and Maple to Obtain Chemical Equations". *J. Chem. Educ.*, **74**:1369–1371, 1997.

[40] Spencer, N. D., and C. J. Pereira. "Partial Oxidation of CH_4 to HCHO over a Mo_3-SiO_2 Catalyst: A Kinetic Study". *AICHE J.*, **33**:1808–1812, 1987.

[41] Stout, R. "Redox Challenges". *J. Chem. Educ.*, **72**:1125, 1995.

[42] Swinnerton, J. W., and W. W. Miller. "Use of a Digital Computer for Solving a Complex Chemical Equilibrium". *J. Chem. Educ.*, **36**:485–489, 1959.

[43] Vaidyanathan, K., and L. K. Doraiswamy. "Controlling Mechanisms in Benzene Oxidation". *Chem. Eng. Sci.*, **23**:537–550, June 1968.

[44] E. Weltin. "Let a Computer Balance Your Chemical Equations and Determine the Number of Independent Reactions". *J. Chem. Educ.*, **71**:295–297, 1994.

[45] D. J. Wink. "The Use of Matrix Inversion in Spreadsheet Programs to Obtain Chemical Equations". *J. Chem. Educ.*, **71**:490–492, 1994.

Acknowledgements

The authors gratefully acknowledge the following beta-testers for providing valuable feedback on the material of this tutorial and on the web site at http://www.chemical-stoichiomietry.net: G. Bjedov (Purdue), W. Seider and A. Ciric (Penn), E. Weltin (Vermont), and D. Wink (Illinois at Chicago).

Financial assistance has been received from the Natural Sciences and Engineering Research Council of Canada; and from the Department of Mathematics and Statistics and the Office of the Dean, College of Physical and Engineering Science, University of Guelph.