A New Approach to Balancing Chemical Equations

by

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Explanatory Note. In what follows, a solution is given of *Problem* 71-25*, which appeared in the Problems and Solutions section of *SIAM Review*, 13 (1971), p. 571. For the reader's convenience, the full statement of the problem is reproduced below.

Problem 71-25*, *Balancing Chemical Equations*, by Michael Jones (University of Dallas).

Suppose that $\boldsymbol{A}$ and $\boldsymbol{B}$ are $p \times n$ and $p \times m$ matrices, respectively, with non-negative entries. Give necessary and sufficient conditions such that the matrix-vector equation $\boldsymbol{Ax} = \boldsymbol{By}$ has positive solutions. If possible, find explicit expressions for $\boldsymbol{x}$ and $\boldsymbol{y}$. This problem had arisen in the attempt to formulate a general method of balancing chemical equations (see R. Crocker, *Application of Diophantine equations to problems in chemistry*, J. Chem. Educ., 45 (1968), pp. 731-733).

Solution of the Problem. Throughout, the set of $m \times n$ matrices over the reals will be denoted by $\mathbb{R}^{m\times n}$. A short solution of the above problem is given by the following theorem.

Theorem. *Let $\boldsymbol{A} \in \mathbb{R}^{p\times n}$ and $\boldsymbol{B} \in \mathbb{R}^{p\times m}$. A g-inverse of $\boldsymbol{A} \in \mathbb{R}^{p\times n}$ is any matrix $\boldsymbol{A}^-$ such that $\boldsymbol{AA}^-\boldsymbol{A} = \boldsymbol{A}$. The linear matrix equation*

$$\boldsymbol{Ax} = \boldsymbol{By} \tag{1}$$

is consistent if and only if for some $\boldsymbol{A}^-$,

$$\boldsymbol{Gy} = \boldsymbol{0}, \tag{2}$$

where

$$\boldsymbol{G} = (\boldsymbol{I} - \boldsymbol{AA}^-)\boldsymbol{B}. \tag{3}$$

If this is the case, a representation of the general solution is

$$\boldsymbol{y} = (\boldsymbol{I} - \boldsymbol{G}^-\boldsymbol{G})\boldsymbol{u} \tag{4}$$

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and

$$\boldsymbol{x} = \boldsymbol{A}^{-}\boldsymbol{B}\boldsymbol{y} + (\boldsymbol{I} - \boldsymbol{A}^{-}\boldsymbol{A})\boldsymbol{v}, \tag{5}$$

with arbitrary vectors $\boldsymbol{u} \in \mathbb{R}^{m\times 1}$ *and* $\boldsymbol{v} \in \mathbb{R}^{n\times 1}$*.*

Proof. Matrix equation (1) is consistent if and only if there exist vectors $\boldsymbol{x} \in \mathbb{R}^{n\times 1}$ and $\boldsymbol{y} \in \mathbb{R}^{m\times 1}$ such that

$$\boldsymbol{A}\boldsymbol{x} - \boldsymbol{B}\boldsymbol{y} = \boldsymbol{0}. \tag{6}$$

From (5) we have $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{A}^{-}\boldsymbol{B}\boldsymbol{y}$, since $\boldsymbol{A}(\boldsymbol{I} - \boldsymbol{A}^{-}\boldsymbol{A}) = \boldsymbol{0}$. Thus, from (6) follows

$$\boldsymbol{A}\boldsymbol{x} - \boldsymbol{B}\boldsymbol{y} = \boldsymbol{A}\boldsymbol{A}^{-}\boldsymbol{B}\boldsymbol{y} - \boldsymbol{B}\boldsymbol{y} = -\boldsymbol{G}\boldsymbol{y}, \tag{7}$$

in view of (3). On the other hand, from (4) it follows that

$$\boldsymbol{G}\boldsymbol{y} = \boldsymbol{G}(\boldsymbol{I} - \boldsymbol{G}^{-}\boldsymbol{G})\boldsymbol{u} = \boldsymbol{0}, \tag{8}$$

in view of $\boldsymbol{G} = \boldsymbol{G}\boldsymbol{G}^{-}\boldsymbol{G}$. Then (1) follows from (8) and (7). □

Remark 1. By the above theorem, the long-standing problem of balancing chemical equations in general form is solved.

Remark 2. The theorem proved here gives *a completely new general method*. It generalizes all known results for balancing chemical equations cited chronologically in references [1]–[125].

REFERENCES

[1] J. Bottommley, Note on a method for determining the coefficients in chemical equations, Chem. News, 37 (1878), pp. 110-111.

[2] O. C. Johnson, Negative bonds and rule for balancing equations, Chem. News, 42 (1880), p. 51.

[3] W. J. Karslake, Balancing of ionic chemical equations, Chem. News, 66 (1907), pp. 41-43.

[4] H. H. Willard, The preparation of perchloric acid, J. Am. Chem. Soc., 34 (1912), pp. 1480 - 1485.

[5] J. A. E. Zimmermann, The value of teaching valence prior to balancing chemical equations, J. Chem. Educ., 2 (1925), pp. 383-385.

[6] M. A. Griggs and M. E. Warner, Applications of modern valence theories to some inorganic chemical reactions, J. Chem. Educ., 3 (1926), pp. 425-431.

[7] J. H. Simons, Chemical equations, J. Chem. Educ., 3 (1926), pp. 1305-1312.

[8] L. J. Waldbauer and W. E. Thurn, Notes on the electron method of teaching oxidation and reduction, J. Chem. Educ., 3 (1926), pp. 1430-1431.

[9] E. R. Jette and V. K. La Mer, The balancing of oxidation-reduction equations. I, J. Chem. Educ., 4 (1927), pp. 1021-1030.

[10] E. R. Jette and V. K. La Mer, The balancing of oxidation-reduction equations. II, J. Chem. Educ., 4 (1927), pp. 1158-1167.

[11] W. T. Hall, Oxidation-reduction equations, J. Chem. Educ., 6 (1929), pp. 479-485.

[12] O. Reinmuth, The structure of matter, VII: Application of the electronic theory to oxidation-reduction, J. Chem. Educ., 6 (1929), pp. 527-535.

[13] B. Park, A rational method for balancing exceptional chemical equations, J. Chem. Educ., 6 (1929), pp. 1136-1139.

[14] S. R. Brinkley, Typical oxidation-reduction reactions in general chemistry, J. Chem. Educ., 6 (1929), pp. 1894-1904.

[15] O. Reinmuth, The structure of mater: Balancing oxidation-reduction equations, J. Chem. Educ., 7 (1930), pp. 1181-1184.

[16] O. Reinmuth, Oxidation-reduction equations, J. Chem. Educ., 7 (1930), pp. 1689-1693.

[17] A. W. S. Endslow, Balancing chemical equations, J. Chem. Educ., 8 (1931), p. 2453.

[18] L. Scheflan, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 358-359.

[19] J. Kendall, Balancing chemical equations, J. Chem. Educ., 9 (1932), p. 360.

[20] A. R. Clark, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 360-361.

[21] N. Dietz, Jr., Balancing chemical equations, J. Chem. Educ., 9 (1932), p. 361.

[22] E. Otto, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 361-363.

[23] B. Menschutkin, Balancing chemical equations, J. Chem. Educ., 9 (1932), p. 560.

[24] O. Slotterbeck, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 751-752.

[25] B. W. Peet, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 752-753.

[26] L. Lehrman, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 944-945.

[27] G. Wernimont, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 1124-1125.

[28] L. Lehrman, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 1125-1126.

[29] J. H. Melville, Balancing chemical equations, J. Chem. Educ., 9 (1932), pp. 1299-1301.

[30] F. W. Smith, Balancing chemical equations, J. Chem. Educ., 10 (1933), p. 250.

[31] H. C. McNeil, Balancing chemical equations, J. Chem. Educ., 10 (1933), p. 707.

[32] H. G. Deming, Balancing equations algebraically, J. Chem. Educ., 11 (1934), p. 125.

[33] C. W. Bennett, Balancing equations by the valence-change method, J. Chem. Educ., 12 (1935), pp. 189-192.

[34] K. B. Morris, The balancing of oxidation-reduction equations, J. Chem. Educ., 15 (1938), pp. 538-540.

[35] O. F. Steinbach, Non-stoichiometric equations, J. Chem. Educ., 21 (1944), p. 66, p. 69.

[36] W. T. Hall, Balancing chemical equations, J. Chem. Educ., 21 (1944), pp. 201-202.

[37] A. Lehrman, Balancing chemical equations, J. Chem. Educ., 21 (1944), pp. 202-203.

[38] Ch. H. Stone, The teaching equations, J. Chem. Educ., 21 (1944), pp. 550-551.

[39] A. Porges, A question of balancing, J. Chem. Educ., 22 (1945), pp. 266-267.

[40] W. C. McGavock, Non-stoichiometric equations, J. Chem. Educ., 22 (1945), pp. 269-270.

[41] C. A. Wanderwerf, A. W. Davidson, and H. H. Sisler, Oxidation-reduction: A re-evaluation, J. Chem. Educ., 22 (1945), pp. 450-456.

[42] A. Standen, Some simple balancing, J. Chem. Educ., 22 (1945), pp. 461-462.

[43] C. A. Wanderwerf, A consistent treatment of oxidation-reduction, J. Chem. Educ., 25 (1948), pp. 547-551.

[44] G. W. Bennett, Otis Coe Johnson and redox equations, J. Chem. Educ., 31 (1954), pp. 157-158.

[45] G. W. Bennett, Material balances and redox equations, J. Chem. Educ., 31 (1954), pp. 324-325.

[46] K. L. Loekwood, Redox revisited, J. Chem. Educ., 38 (1961), pp. 326-329.

[47] R. Haas and K. H. Gayer, Balancing ionic equations by the method of undetermined coefficients, J. Chem. Educ., 39 (1962), pp. 537-538.

[48] R. Aris and R. H. S. Math, Independence of chemical reactions, Ind. Eng. Chem. Fundam., 2 (1963), pp. 90-94.

[49] D. R. Swayze, Balancing chemical equations, J. Chem. Educ., 40 (1963), pp. 269-270.

[50] H. W. Ferguson, Algebra for balancing redox reactions, Chemistry, 40 (2) (1967), pp. 18-20.

[51] V. L. Fabishak, Matrix method for balancing chemical equations, Chemistry, 40 (11) (1967), pp. 18-21.

[52] G. N. Copley, Linear algebra of chemical formulas and equations, Chemistry, 41 (9) (1967), pp. 22-27.

[53] R. Crocker, Application of Diophantine equations to problems in chemistry, J. Chem. Educ., 45 (1968), pp. 731-733.

[54] G. N. Copley, Algebra and chemical equations, J. Chem. Educ., 46 (1969), p. 699.

[55] R. Crocker, Algebra and chemical equations, J. Chem. Educ., 46 (1969), p. 699.

[56] J. P. Brown, L. P. Brown, and R. M. Redd, A computer program for balancing chemical equations, J. Chem. Educ., 49 (1972), p. 754.

[57] G. Van Cleave, Redox?, Chem 13 News, 62 (1974), p. 12.

[58] D. A. Robinson, Redox?, Chem 13 News, 64 (1974), p. 7.

[59] D. R. Schneider and G. V. Reklaitis, On material balances for chemically reacting system, Chem. Eng. Sci., 30 (1975), pp. 243-247.

[60] A. I. Rosen, A computer program designed to balance inorganic chemical equations, J. Chem. Educ., 54 (1977), p. 704.

[61] D. Kolb, The chemical equation, Part II: Oxidation-reduction reactions, J. Chem. Educ., 55 (1978), pp. 326-331.

[62] S. A. Carrano, Balancing an atypical redox equation, J. Chem. Educ., 55 (1978), p. 382.

[63] E. V. Krishnamurthy, Generalized matrix inverse for automatic balancing of chemical equations, Int. J. Math. Educ. Sci. Technol., 9 (1978), pp. 323-328.

[64] S. Z. Goldberg, EQUBAL - A computer program for balancing chemical equations, J. Chem. Educ., 55 (1978), pp. 532.

[65] D. Kolb, More on balancing redox equations, J. Chem. Educ., 56 (1979), pp. 181-184.

[66] D. Kolb, Balancing complex redox equations by inspection, J. Chem. Educ., 58 (1981), pp. 642-645.

[67] E. Pernicone, Method for balancing redox reactions containing hydroxyl ions, J. Chem. Educ., 58 (1981), p. 966.

[68] J. H. Kennedy, Balancing chemical equations with a calculator, J. Chem. Educ., 59 (1982), pp. 523-524.

[69] G. R. Blakley, Chemical equation balancing: A general method which is quick, simple, and has unexpected applications, J. Chem. Educ., 59 (1982), pp. 728-734.

[70] R. A. Alberty, Balancing complex chemical equations using a hand-held calculator, J. Chem. Educ., 60 (1983), pp. 102-103.

[71] F. M. Stark, Note to: Method for balancing redox reactions containing hydroxyl ions, J. Chem. Educ., 61 (1984), p. 476.

[72] M. Niaz and A. E. Lawson, Balancing chemical equations: The role of developmental level and mental capacity, J. Res. Sci. Teach., 22 (1985), pp. 41-51.

[73] D. F. Swinehart, More on chemical reaction balancing, J. Chem. Educ., 62 (1985), p. 55.

[74] W. L. Yarroch, Student understanding of chemical equation balancing, J. Res. Sci. Teach., 22 (1985), pp. 449-459.

[75] S. K. Porter, How should equation balancing be taught?, J. Chem. Educ., 62 (1985), pp. 507-508.

[76] W. Loercher, Balancing chemical equations with Commodore 64, J. Chem. Educ., 63 (1986), p. 74.

[77] S. C. Das, A mathematical method of balancing a chemical equation, Int. J. Math. Educ. Sci. Technol., 17 (1986), pp. 191-200.

[78] W. Harjadi, A simple method of chemical reaction balancing, J. Chem. Educ., 63 (1986), pp. 978-979.

[79] D. W. Brooks, What next?, J. Chem. Educ., 64 (1987), pp. 53-54.

[80] A. García, A new method to balance chemical equations, J. Chem. Educ., 64 (1987), pp. 247-248.

[81] W. B. Jensen, Unbalanced chemical equations, J. Chem. Educ., 64 (1987), p. 646.

[82] W. C. Herndon, On balancing chemical equations, Int. J. Math. Educ. Sci. Technol., 18 (1987), pp. 745-746.

[83] S. C. Das, On balancing chemical equations, Int. J. Math. Educ. Sci. Technol., 18 (1987), pp. 746-747.

[84] E. L. Cheluget and R. W. Missen, Computer calculation of ionic equilibria using species - or reaction-related thermodynamic data, J. Phys. Chem., 91 (1987), pp. 2428-2432.

[85] R. W. Missen and W. R. Smith, A question of basic chemical literacy?, J. Chem. Educ., 66 (1989), pp. 217-218.

[86] O. Barberá, Ajuste de ecuaciones qumicas: ¿por qué usar reglas arbitrarias y hechos ficticios?, Ens. Cien., 8 (1990), pp. 85-88.

[87] I. B. Risteski, The new algebraic criterions to even out the chemical reactions, 22nd Oct. Meeting of Min. & Metall., Collection of Papers, Oct. 1-2, Bor 1990, pp. 313-318.

[88] J. M. Campanario and R. Ballesteros, Ajuste de ecuaciones qumicas: un enunciado poco afortunado para un problema ya resuelto, Ens. Cien., 9 (1991), pp. 205-207.

[89] R. W. Missen and W. R. Smith, The permanganate-peroxide reaction, J. Chem. Educ., 67 (1990), pp. 876-877.

[90] R. A. Alberty, Chemical equations are actually matrix equations, J. Chem. Educ., 68 (1991), p. 984.

[91] C. A. L. Filgueiras, Balancing a chemical equation: What does it mean? J. Chem. Educ., 69 (1992), pp. 276-277.

[92] R. A. Alberty, Conversion of chemical equations to biochemical equations, J. Chem. Educ., 69 (1992), p. 493.

[93] D. D. Kumar, Hyperequation, The Agora, 3 (1993), pp. 8-9.

[94] S. Toby, Ambiguities in balancing chemical equations, J. Chem. Educ., 71 (1994), p. 270.

[95] E. Weltin, Let a computer balance your chemical equations and determine the number of independent reactions, J. Chem. Educ., 71 (1994), pp. 295-297.

[96] D. J. Wink, The use of matrix inversion in spreadsheet programs to obtain chemical equation, J. Chem. Educ., 71 (1994), pp. 490-492.

[97] J. M. Campanario, Automatic "balancing" of chemical equations, Computers Chem., 19 (1995), pp. 85-90.

[98] D. W. Brooks, Retrospective tutoring, J. Chem. Educ., 72 (1995), pp. 233-236.

[99] M. E. Cardinali, Double disproportions, J. Chem. Educ., 72 (1995), p. 716.

[100] R. Subramanian, N. K. Goh, and L. S. Chia, The relationship between the number of elements and the number of independent equations of elemental balance in inorganic chemical equations, J. Chem. Educ., 72 (1995), p. 894.

[101] R. Stout, Redox challenges: Good times for puzzle fanatics, J. Chem. Educ., 72 (1995), p. 1125.

[102] A. Garritz and C. Rincón, Capricho valenciano (I): ¿Tiene alguna interpretación fisica el método de balanceo por números de oxidación?, Educ. Quím., 7 (1996), pp. 190-195.

[103] O. G. Ludwig, On balancing "redox challenges", J. Chem. Educ., 73 (1996), p. 507.

[104] D. M. Hart, Redox challenges, J. Chem. Educ., 73 (1996), p. A226.

[105] N. S. Zaugg, Redox challenges, J. Chem. Educ., 73 (1996), pp. A226-A227.

[106] R. Stout, Redox challenges, J. Chem. Educ., 73 (1996), p. A227.

[107] L. A. Ferguson, How do I balance thee? ... Let me count the ways?, J. Chem. Educ., 73 (1996), p. 1129.

[108] M. C. Hernández, Balanceo de ecuaciones qumicas mediante computadora, Educ. Quím., 8 (1997), pp. 56-62.

[109] J. A. Olson, An analysis of the algebraic method for balancing chemical reactions, J. Chem. Educ., 74 (1997), pp. 538-542.

[110] D. M. Hart, Corrections, J. Chem. Educ., 74 (1997), p. 1256.

[111] R. Nelson, Redox challenges, J. Chem. Educ., 74 (1997), p. 1256.

[112] A. Sobkowiak, Balancing chemical equations, J. Chem. Educ., 74 (1997), pp. 1256-1257.

[113] Z. Tóth, On balancing "redox challenges" by unconventional oxidation numbers, J. Chem. Educ., 74 (1997), p. 1270.

[114] A. A. Woolf, Unconventional oxidation numbers, J. Chem. Educ., 74 (1997), p. 1270.

[115] O. Ludwig, Balancing chemical equations, J. Chem. Educ., 74 (1997), pp. 1270-1271.

[116] W. A. Freeman, N. K. Goh, L. S. Chia, D. M. Hart, E. A. Lucas, D. J. Peery, R. Subramanian, and M. J. ten Hoor, How do I balance thee? ... Let me count the ways?, J. Chem. Educ., 74 (1997), p. 1271.

[117] W. C. Herndon, On balancing chemical equations: Past and present, J. Chem. Educ., 74 (1997), pp. 1359-1362.

[118] Z. Tóth, Balancing chemical equations by inspection, J. Chem. Educ., 74 (1997), pp. 1363-1364.

[119] Ch. Guo, A new inspection method for balancing redox equations, J. Chem. Educ., 74 (1997), pp. 1365-1366.

[120] M. J. ten Hoor, Redox balancing without puzzling, J. Chem. Educ. 74, (1997), pp. 1367-1368.

[121] P. Glaister, A challenging balance, J. Chem. Educ., 74 (1997), p. 1368.

[122] W. R. Smith and R. W. Missen, Using Mathematica and Maple to obtain chemical equations, J. Chem. Educ., 74 (1997), pp. 1369-1371.

[123] K. Balasubramanian, Linear variational Diophantine techniques in mass balance of chemical reactions, J. Math. Chem., 30 (2001), pp. 219-225.

[124] D. D. Kumar, Computer applications in balancing chemical equations, J. Sci. Educ. Technol., 10 (2001), pp. 347-350.

[125] S. K. Sen, H. Agarwal, and S. Sen, Chemical equations balancing: An integer programming approach, Math. Comput. Modelling, 44 (2006), pp. 678-691.