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pH and Conductivity of Sodium Phosphate Solutions

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March 1979

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ABSTRACT

The purpose of this paper is to describe a computer program for the calculation of the pH and conductivity of sodium phosphate solutions over the phosphate concentration range of 1 to 10000 ppm and sodium to phosphate molar ratios of approximately 2 to 3. pH can be calculated over the temperature range of 0 to 300°C; conductivities can be calculated over the temperature range of 0 to 50°C.

Calculated values of pH and conductivity are compared to measured values and found to be in excellent agreement.

Several practical uses for the computer program are discussed.

pH and Conductivity of Sodium Phosphate Solutions

I. Introduction

The purpose of this paper is to demonstrate how to calculate the pH and conductivity of sodium phosphate solutions, compare the calculated values against measured values, and show various practical applications for the calculations. The computer program was written in BASIC language for a DEC-10 computer and contains temperature dependent parameters such as the ionization constants for phosphoric acid and water, the dielectric constant, density and viscosity of water, and the molar ionic conductivities of the various ions present in phosphate solutions. The temperature dependent parameters used in the calculation of pH are valid over the temperature range of 0 to 300°C. However, the temperature dependent equations for the molar ionic conductivities of the ions are valid only over the temperature range of 0 to 50°C and, consequently, the calculated conductivities may not be valid at temperatures higher than 50°C.

II. Calculations of pH

The equations representing any chemical system in equilibrium must meet the following conditions:

1. All equilibria existing in the system must be satisfied.
2. Matter must be conserved.
3. Electrical neutrality must be maintained.

The equilibria which must be satisfied consist of the ionization equilibria equations for phosphoric acid and water:

$$K_1 = \frac{a_{H^+} a_{H_2PO_4^-}}{a_{H_3PO_4}} = \frac{[H^+][H_2PO_4^-]\gamma_1^2}{[H_3PO_4]} \quad (1)$$

$$K_2 = \frac{a_{H^+} a_{HPO_4^{2-}}}{a_{H_2PO_4^-}} = \frac{[H^+][HPO_4^{2-}]\gamma_2}{[H_2PO_4^-]} \quad (2)$$

$$K_3 = \frac{a_{H^+} a_{PO_4^{3-}}}{a_{HPO_4^{2-}}} = \frac{[H^+][PO_4^{3-}]}{[HPO_4^{2-}]} \frac{\gamma_1 \gamma_3}{\gamma_2} \quad (3)$$

$$K = \frac{a_{H^+} a_{OH^-}}{1} = [H^+][OH^-] \gamma_1^2 \quad (4)$$

The material balance equation is:

$$T_1 = [H_3PO_4] + [H_2PO_4^-] + [HPO_4^{2-}] + [PO_4^{3-}] \quad (5)$$

The electrical neutrality equation is:

$$[Na^+] + [H^+] = [OH^-] + [H_2PO_4^-] + 2[HPO_4^{2-}] + 3[PO_4^{3-}]$$

In the above equations, the a 's represent activities of the various species; the bracketed terms represent molar concentrations; the K 's represent equilibrium constants; the γ 's represent activity coefficients for the uni (1), di (2), and tri (3) valent ions; and T_1 represents the total phosphate (PO_4) molar concentration in the solution.

Assuming, for the moment, that the values for the γ 's are known, the above six equations contain eight unknowns: $[H_3PO_4]$, $[H^+]$, $[H_2PO_4^-]$, $[HPO_4^{2-}]$, $[PO_4^{3-}]$, $[OH^-]$, T_1 , and $[Na^+]$. By specifying the composition of the solution, i.e., specifying T_1 and $[Na^+]$, the six equations can be solved for the six unknowns. The method used to solve for the unknowns consisted of:

1. Assigning the value of 1.0 to each activity coefficient,
2. Solving for $[H_3PO_4]$, $[H_2PO_4^-]$, and $[HPO_4^{2-}]$ in terms of the ionization constants, $[PO_4^{3-}]$ and $[OH^-]$ using equations (1) through (4),
3. Solving for $[PO_4^{3-}]$ in terms of the ionization constants, T_1 , and $[OH^-]$ by substituting the solutions from step 2 into equation (5),

4. Solving for $[H_2PO_4^-]$ and $[HPO_4^{=}]$ in terms of ionization constants, T_1 , and $[OH^-]$ by substituting the value for $[PO_4^{=}]$ from step 3 into the equations for $[H_2PO_4^-]$ and $[HPO_4^{=}]$ found in step 2,
5. Solving for $[OH^-]$ in terms of $[Na^+]$, T_1 , and the ionization constants by substituting the values for $[H_2PO_4^-]$, $[HPO_4^{=}]$, and $[PO_4^{=}]$ found in steps 3 and 4, along with $[H^+] = [OH^-] \gamma_1^2 / K$, into equation (6).
The equation for $[OH^-]$ is:

$$C [OH^-]^5 + C_1 [OH^-]^4 + C_2 [OH^-]^3 + C_3 [OH^-]^2 + C_4 [OH^-] + C_5 = 0 \quad (7)$$

in which

$$C = K_4 K_5 K_6 / K_7^3$$

$$C_1 = \frac{K_4 K_5}{K_7^2} + \frac{3 K_4 K_5 K_6 T_1}{K_7^3} - \frac{K_4 K_5 K_6}{K_7^3} [Na^+]$$

$$C_2 = \frac{K_4}{K_7} + 2 \frac{K_4 K_5 T_1}{K_7^2} - \frac{K_4 K_5}{K_7^2} [Na^+] - \frac{K_4 K_5 K_6}{K_7^2}$$

$$C_3 = 1 + \frac{K_4 T_1}{K_7} - \frac{K_4}{K_7} [Na^+] - \frac{K_4 K_5}{K_7}$$

$$C_4 = - \left[K_4 + [Na^+] \right]$$

$$C_5 = - K_7$$

6. Solving the above polynomial for $[OH^-]$ using the Newton-Raphson method,

7. Solving for the molar concentration of each of the other species by substituting the value for $[\text{OH}^-]$ obtained from step 6 into the equations relating the species to $[\text{OH}^-]$, T_1 , and the ionization constants (see steps 3 and 4),
8. Calculating values for γ_1 , γ_2 , and γ_3 by substituting the concentration values for the various species into the following equation which was obtained from an extension of the Debye-Huckel theory:

$$\ln \gamma_i = - \frac{(Z_i e)^2}{2DkT} \frac{K}{1 + Ka_i} \quad (8)$$

$$K = \left[\frac{4\pi e^2 NS}{1000 DkT} \right]^{1/2}$$

$$S = \sum C_i Z_i^2 = [\text{Na}^+] + [\text{H}^+] + [\text{OH}^-] + [\text{H}_2\text{PO}_4^-] + 4 [\text{HPO}_4^{2-}] + 9 [\text{PO}_4^{3-}]$$

in which

Z_i = valence of the i th ion

e = electronic charge = 4.80223×10^{-10} esu

D = dielectric constant of the solution

k = Boltzmann's constant = 6.62377×10^{-27} erg-sec/molecule

T = absolute temperature ($^{\circ}\text{K}$)

a_i = minimum average distance to which ions, both positive and negative, can approach one another, a_i was chosen to be 4 angstroms

N = Avagadro's number

C_i = molar concentration

9. Comparing the values for each of the calculated γ 's with the assumed value of 1. If the calculated values differ by more than an arbitrary percentage (we used 0.1 percent), the calculated values were substituted into equations (1) through (4) and steps 2 through 9 were repeated. The iteration process was continued until the new calculated value for each γ was within 0.1 percent of the previous calculated value,
10. Calculating pH using

$$\text{pH} = -\log a_{\text{H}^+} = -\log \gamma_1 [\text{H}^+]$$

and the final calculated γ_1 and $[\text{H}^+]$

The values for the ionization constants for phosphoric acid and water used in the calculations were:

$$\begin{aligned} \ln K_1 = & \frac{2.85829 \times 10^4}{T} - 501.5113 - 0.094568T + 78.9595 \ln T \\ & - \frac{18.654 \times 10^5}{T^2} \end{aligned} \quad (9)$$

$$\begin{aligned} \ln K_2 = & \frac{2.7434 \times 10^4}{T} - 485.0409 - 0.0938T + 75.0608 \ln T \\ & - \frac{20.6675 \times 10^5}{T^2} \end{aligned} \quad (10)$$

$$\ln K_3 = \frac{16482.1}{T} - 858.75 - 0.2883T + 151.09 \ln T \quad (11)$$

$$\log K = - \frac{5242.39}{T} + 35.3944 - 0.00853T - 11.8261 \log T \quad (12)$$

in which T is expressed in degrees Kelvin. Equation (9) was obtained by adding equation (12) for the ionization constant of water to an equation given in Reference (1) which describes, as a function of temperature, the equilibrium constant for:

Equation (10) was obtained in a similar manner using an equation in Reference (1) which describes the change in the equilibrium constant with temperature for the reaction:

Equation (11) was obtained by subtracting equation (13) from equation (12). Equation (13) describes the effect of temperature on the hydrolysis reaction:

Data from N. C. Treloar, "Raman Study of Phosphate Equilibria in Aqueous Solutions from 25 to 150°C" Central Electricity Research Laboratories, Leatherhead, Surry, England and the method of least squares were used to determine equation (13) which is:

$$\ln Q = - \frac{28553.1}{T} + 940.25 + 0.2687T - 162.92 \ln T \quad (13)$$

Equation (12), which describes the change in the ionization constant of water with temperature, was obtained from Reference (2).

Values for the ionization constants for phosphoric acid and water as a function of temperature are shown in Table I.

Table I
Values for the Ionization Constants of Phosphoric Acid and
Water over the Temperature Range 0 to 300°C

TEMP. °C	K1	K2	K3	K
0	8.75541E-3	4.88624E-8	1.48262E-13	1.14653E-15
25	7.12153E-3	6.32094E-8	3.89001E-13	1.01283E-14
50	5.26646E-3	6.56903E-8	7.68901E-13	5.48211E-14
75	3.67965E-3	5.89878E-8	1.13406E-12	2.03165E-13
100	2.47662E-3	4.77721E-8	1.25115E-12	5.58751E-13
125	1.62088E-3	3.58055E-8	1.04177E-12	1.21063E-12
150	1.03587E-3	2.52358E-8	6.62738E-13	2.16206E-12
175	6.47373E-4	1.68950E-8	3.26578E-13	3.29531E-12
200	3.95683E-4	1.08143E-8	1.26426E-13	4.40458E-12
225	2.36411E-4	6.64691E-9	3.89893E-14	5.27516E-12
250	1.37980E-4	3.93488E-9	9.70862E-15	5.75939E-12
275	7.86085E-5	2.24833E-9	1.97689E-15	5.81287E-12
300	0.0000436879	1.24198E-9	3.33135E-16	5.48568E-12

The equations for the change in the **dielectric constant of water** with temperature and the change in the density of water with temperature were obtained from References (3) and (4), respectively. These equations were:

$$D_6 = \frac{5321}{T} + 233.76 - 0.9297 T + 1.417 \times 10^{-3} T^2 - 8.292 \times 10^{-7} T^3 \quad (14)$$

and

$$D_2 = 1 - \frac{(t - 3.9863)^2 (t + 288.9414)}{508929.2 (t + 68.12963)} \quad (15)$$

in which t is degrees centigrade.

III. Calculation of Conductivity

By definition, conductivity ($\mu\text{mho/cm}$) is:

$$L (\mu\text{mho/cm}) = (\sum \lambda_j C_j) \times 10^3$$

$$\text{in which } \sum \lambda_j C_j = \lambda_{\text{Na}} [\text{Na}^+] + \lambda_{\text{H}} [\text{H}^+] + \lambda_{\text{OH}} [\text{OH}^-] + \lambda_{\text{H}_2\text{PO}_4} [\text{H}_2\text{PO}_4^-] \\ + \lambda_{\text{HPO}_4} [\text{HPO}_4^{=}] + \lambda_{\text{PO}_4} [\text{PO}_4^{\equiv}] \quad (16)$$

and the λ_j 's are the ionic molar conductivities at the C_j concentrations.

The $\lambda_j C_j$ values for the sodium, hydrogen, and **hydroxyl** ions can be calculated at various temperatures from the relationships, Reference (6):

$$\lambda_{\text{Na}}^{\circ} = 50.11 (1 + 0.0209 (t - 25)) \quad (17)$$

$$\lambda_{\text{OH}}^{\circ} = 198 (1 + .0160 (t - 25)) \quad (18)$$

$$\lambda_{\text{H}}^{\circ} = 349.8 (1 + .0142 (t - 25)) \quad (19)$$

the concentrations obtained from the pH calculation, and the Onsager-Fuoss equation, Reference (6):

$$\lambda_j = \lambda_j^0 - S_1 \sum C_i Z_i^2 \quad (20)$$

$$S_1 = \frac{5.802 \times 10^5 \lambda_j^0}{(DT)^{3/2}} + \frac{29.16 (Z_j)}{\eta (DT)^{1/2}}$$

in which

λ_j = molar ionic conductivity of the j-th ion at a concentration Ci

λ_j^0 = limiting molar ionic conductivity of the j-th ion at infinite dilution

Z_j = charge on the j-th ion

D = dielectric constant of the solution at temperature T ($^{\circ}$ K)

η = viscosity of the solution at temperature T ($^{\circ}$ K). The viscosity of water as a function of temperature was obtained by the method of least squares using data given in Reference (4). The equation used was:

$$\ln \eta = \frac{7738.88}{T} - 181.278 - .0296488T + 27.9854 \ln T$$

$\sum C_i Z_i^2$ = sum of the product of the molar concentrations and ionic charges squared for all of the ions in the solution

The molar ionic conductivity values for the $H_2PO_4^-$, HPO_4^{2-} or PO_4^{3-} are not known. The contributions of the phosphate ions to the conductivity of a sodium phosphate solution were estimated as follows:

- (1) The conductivity of a sodium phosphate solution containing 250 ppm PO_4 with a Na/ PO_4 molar ratio of 2.30, was measured over the temperature range of 15 to 40 $^{\circ}$ C. This particular concentration was chosen for measurement since it represents a typical boiler water concentration used in many plants. The conductivity of this solution is the same as that shown by equation (16). From previous calculations of pH, it is known that the major ions in boiler water solutions are the Na^+ , OH^- , and HPO_4^{2-} . Approximate molar concentrations are:

<u>Ion</u>	<u>Molar Concentration</u>
Na^+	3.5×10^{-3}
OH^-	3×10^{-4}
H_2PO_4^-	6×10^{-7}
$\text{HPO}_4^{=}$	1×10^{-3}
$\text{PO}_4^{\equiv}$	3×10^{-5}
H^+	3×10^{-11}

- (2) Since the concentrations of the H^+ and H_2PO_4^- are quite small compared to the other ions, equation (16) was rewritten deleting these ions:

$$L \times 10^{-3} - \left[\lambda \text{Na} [\text{Na}^+] + \lambda \text{OH} [\text{OH}^-] \right] = \lambda \text{HPO}_4 [\text{HPO}_4^{=}] + \lambda \text{PO}_4 [\text{PO}_4^{\equiv}] \quad (21)$$

The $[\text{PO}_4^{\equiv}]$ can be related to $[\text{HPO}_4^{=}]$ from equations (3) and (4) to give:

$$[\text{PO}_4^{\equiv}] = \frac{K_3 \gamma_1 \gamma_2 [\text{OH}^-] [\text{HPO}_4^{=}]}{K \gamma_3} \quad (22)$$

Substituting equation (22) into equation (21) and rearranging gives:

$$\frac{L \times 10^{-3} - \left[\lambda \text{Na} [\text{Na}^+] + \lambda \text{OH} [\text{OH}^-] \right]}{[\text{HPO}_4^{=}]} = \lambda \text{HPO}_4 + \frac{\lambda \text{PO}_4 K_3 \gamma_1 \gamma_2 [\text{OH}^-]}{K \gamma_3} = Y \quad (23)$$

The right side of equation (23) is the molar ionic conductivity contribution of the phosphate ions, labeled Y.

- (3) Plotting the left side of equation (23) vs temperature gives a straight line which has the relationship:

$$Y_t = Y_{25} (1 + a (t-25)) \quad (24)$$

in which $Y_{25} = 124.7$ and $a = 0.0225$

- (4) Therefore, the conductivity of a sodium phosphate solution can be expressed as:

$$L = \left[\lambda Na [Na^+] + \lambda H [H^+] + \lambda OH [OH^-] + Y [HPO_4^{2-}] \right] \times 10^3 \quad (25)$$

IV. Computer Program

The input, output, and a sample problem from the computer program used to calculate the pH and conductivity of sodium phosphate solutions written in the BASIC language is shown below. Copies of this program may be obtained by domestic users from:

National Energy Software Center
 Att: Mrs. Margaret Butler
 Argonne National Laboratory
 9700 South Cass Avenue
 Argonne, Illinois 60440

A. Input and Output

Input required for the determination of the pH and conductivity of a sodium phosphate solution consists of: (1) the sodium/phosphate molar ratio or range of molar ratios, (2) ppm total phosphate or range of phosphate concentrations, and (3) temperature or range of temperatures of the solution in degrees Celcius.

The value of any parameter in the program may be printed as output as a function of sodium phosphate composition and solution temperature using an appropriate print statement.

For example, the values for the uni-, di-, and tri-valent activity coefficients may be printed as a function of sodium phosphate composition and solution temperature or the ionization constants for phosphoric acid and water may be printed as a function of temperature (See Table I).

In addition, titration curves (titrating a particular sodium phosphate solution with an acid) can be obtained. Required input for a titration curve are: sodium/phosphate molar ration, ppm total phosphate, volume of solution titrated, normality of acid titer, and volume of titer added during the titration.

The effect of carbon dioxide absorption or other impurities on the pH of sodium phosphate solutions can be determined by modifying the program to incorporate the appropriate equilibrium constants, material balance, and electrical neutrality equations and by changing the ionic strength equation to incorporate the presence of the impurity. To determine the effect of carbon dioxide on pH the above changes result in a seventh order polynomial equation for the hydroxyl ion concentration which is determined by the Newton-Raphson method.

B. Sample Problem

1. Input

```
190 U = 2.0
200 FOR T3 = 50 TO 800 STEP 50
260 I = 25.0
1960 NEXT T3
```

2. Output

RUNINH

NA/PO4	PPM PO4	PH	COND
2	50	8.91017	117.263
2	100	9.04107	232.644
2	150	9.11245	346.985
2	200	9.15985	460.506
2	250	9.19426	573.324
2	300	9.22055	685.52
2	350	9.24131	797.152
2	400	9.25805	908.264
2	450	9.27179	1018.89
2	500	9.28317	1129.06
2	550	9.29268	1238.8
2	600	9.30068	1348.13
2	650	9.30742	1457.07
2	700	9.31312	1565.64
2	750	9.31793	1673.84
2	800	9.322	1781.7

TIME: 2.38 SECS.

V. Plot of pH vs Conductivity as a Function of Total Phosphate and the Na/PO₄ Molar Ratio

Figure 1 was produced using results from the computer program described in Section IV above.

FIGURE I
pH AND CONDUCTIVITY OF PHOSPHATE SOLUTION AT 25°C

VI. Comparison of Calculated pH and Conductivity Values with Measured Values

A. Buffers - The National Bureau of Standards (Reference (7)) has carefully measured the pH of two phosphate buffer solutions over the temperature range of 0 to 50°C.

Tables II and III show a comparison of the measured pH values with the values calculated using the computer program described in Section IV.

Table II
NBS Buffer with Composition 0.025 M Na_2HPO_4 , 0.025 M KH_2PO_4

Temperature (°C)	pH		ΔpH
	Measured	Calculated	(Measured-Calculated)
0	6.984	6.981	+ .003
5	6.951	6.947	+ .004
10	6.923	6.917	+ .006
15	6.900	6.893	+ .007
20	6.881	6.873	+ .008
25	6.865	6.856	+ .009
30	6.853	6.844	+ .009
35	6.844	6.834	+ .010
40	6.838	6.828	+ .010
45	6.834	6.825	+ .009
50	6.833	6.824	+ .009

Table III
NBS Buffer with Composition 0.03043 M Na_2HPO_4 , 0.008695 M KH_2PO_4

Temperature (°C)	pH		ΔpH
	Measured	Calculated	(Measured-Calculated)
0	7.534	7.525	+ .009
5	7.500	7.491	+ .009
10	7.471	7.461	+ .010
15	7.448	7.437	+0.011
20	7.429	7.417	+0.012
25	7.413	7.400	+0.013
30	7.400	7.388	+ .012
35	7.389	7.378	+ .011
40	7.380	7.372	+ .008
45	7.373	7.368	+ .005
50	7.367	7.368	-0.001

- B. pH of Phosphate Solutions - Reference (8) showed figures depicting measured pH values for phosphate solutions ranging in total phosphate from 1 to 10,000 ppm and Na/PO_4 molar ratios of 1.975 to 2.90. In Figures 2 through 11 these measured values* are compared against the calculated values obtained from the computer program. In the figures a circled dot indicates only one data point was obtained; a circled dot containing limits (95 percent confidence interval limits) indicates that duplicate or triplicate measurements were made. The solid line indicates the calculated pH values using the computer program.

In Figures 12 and 13 the measured pH values* are compared against calculated pH values for various phosphate concentrations in 1 M KCl solutions. The Na/PO_4 molar ratio was 2.00 (Figure 12) and 2.30 (Figure 13). The computer program was altered to accommodate the 1 M KCl by changing the ionic strength statement. The ionic strength of the solution is used in calculating the activity coefficients.

Calculated pH values for sodium phosphate solutions at 50°C and a Na/PO_4 molar ratio of 2.50 are compared against measured values* in Figure 14.

As illustrated by the figures the agreement between the measured and calculated values is very good.

- C. Conductivity of Phosphate Solutions - The authors know of no published conductivity measurements of sodium phosphate solutions which have been made to cover the Na/PO_4 molar ratio range from 2.0 to 3.0. However, several hundreds of measurements of the pH and conductivity of various sodium phosphate solutions have been made to estimate the phosphate concentrations in solutions through the use of Figure 1. For example, Figure 1 shows that a sodium phosphate solution with a conductivity of 700 $\mu\text{mho}/\text{cm}$ and a pH of 10.70 has a phosphate concentration of approximately 250 ppm and a Na/PO_4 molar ratio of approximately 2.25. The phosphate concentrations estimated from the pH and conductivity measurements and Figure 1 have been compared to the phosphate concentrations in

*Data obtained from Dr. J. Roesmer, Westinghouse PWR Division, Pittsburgh, PA

FIGURE 2
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 1.975
TEMPERATURE 25°C

FIGURE 3
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.00
TEMPERATURE 25°C

FIGURE 4
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.015
TEMPERATURE 25°C

FIGURE 5
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.02
TEMPERATURE 25°C

pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.109

TEMPERATURE 25°C

FIGURE 8

pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.30

TEMPERATURE 25°C

pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.29

TEMPERATURE 25°C

FIGURE 9

pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO₄ MOLAR RATIO OF 2.47

TEMPERATURE 25°C

FIGURE 10
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO_4 MOLAR RATIO OF 2.6
TEMPERATURE 25°C

FIGURE 11
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO_4 MOLAR RATIO OF 2.9
TEMPERATURE 25°C

FIGURE 12
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO_4 MOLAR RATIO OF 2.00 IN 1M KCl
TEMPERATURE 25°C

FIGURE 13
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO_4 MOLAR RATIO OF 2.30 IN 1M KCl
TEMPERATURE 25°C

FIGURE 14
pH AND PHOSPHATE CONCENTRATION DATA AT A Na/PO_4 MOLAR RATIO OF 2.50
TEMPERATURE 50°C

the solutions determined by (1) preparing the solutions from known amounts of $\text{Na}_3\text{PO}_4 \cdot 12\text{H}_2\text{O}$ and Na_2HPO_4 , (2) using the colorimetric phosphovanadomolybdic acid procedure (Reference (9)), and (3) using the gravimetric magnesium ammonium phosphate procedure (Reference (10)). The pH, conductivity, and phosphate measurements were performed by many different people over a 2 to 4 year period. The comparison shows that the pH/conductivity/Figure 1 method gives phosphate results which are within ± 6 percent of the results obtained from the analytical methods. Thus, it is apparent that the calculated conductivities of sodium phosphate solutions, shown in Figure 1, are quite accurate at least over the phosphate concentration range of 5 to 400 ppm and the Na/PO_4 molar ratio range of 2.0 to 3.0 which are the ranges covered by the many pH and conductivity measurements.

VII. Uses

The computer program has several practical uses:

1. Determination of total phosphate concentration from pH and conductivity measurements.
 2. Calculation of acid titration curves and effect of CO_2 absorption on titration curves.
 3. Quality control of phosphate buffer solutions.
 4. Determination of temperature coefficients for pH and conductivity.
-
- A. Determination of Total Phosphate Concentration from pH and Conductivity Measurements. As shown in Section VI C, the total phosphate concentration in a boiler water phosphate solution can be determined by measurement of the pH and conductivity of the solution and use of Figure 1.
 - B. Calculation of Acid Titration Curves. The computer program can be altered to calculate acid titration curves for phosphate solutions. For example, to calculate a titration curve for the titration of 200 ml of phosphate solution containing 250 ppm total phosphate and a Na/PO_4 molar ratio of 2.6 with 0.210 N HNO_3 , the following changes are made to the program:

Values for the sodium/phosphate molar ratio (2.6), ppm total phosphate (250) are input into the program. Statements are added to the program to incorporate the normality of the acid (.210 N), the volume of the solution (200 ml), and to permit acid increments to be added to the solution titrated. The program statements for the molar concentration of sodium and total phosphate are changed to allow for dilution of the solution by the acid titer and the statement for the ionic strength of the solution is changed to accommodate the concentration of nitrate ion added during the acid titration. Print statements for output of volume of acid and solution pH are incorporated.

Figure 15 shows the results of the calculated titration curve. The volume of acid (ml) required to lower the pH from 9.2 ± 0.2 to 5.0 ± 0.2 is the titration:

The concentration of phosphate (ppm) in the solution is:

$$\text{ppm PO}_4 = \frac{V_{\text{HNO}_3} \times 0.210 \times 94.97 \times 10^3}{200} = 100 V_{\text{HNO}_3}$$

or since $V_{\text{HNO}_3} = 2.5$, $\text{ppm PO}_4 = 250 \text{ ppm}$

The computer program can be further modified to determine the effect of impurities on the acid titration of phosphate solutions. For example, the effect on the titration of absorbing carbon dioxide into a phosphate solution can be determined by: (1) adding to the computer program the equilibrium equations for carbon dioxide:

$$F_1 = \frac{[\text{H}^+][\text{HCO}_3^-]}{[\text{H}_2\text{CO}_3]} \gamma_1^2 \text{ and } F_2 = \frac{[\text{H}^+][\text{CO}_3^{2-}]}{[\text{HCO}_3^-]} \gamma_2 \text{ in which}$$

$$\log F_1 = - \frac{3404.71}{T} + 14.8435 - .03278 T$$

$$\log F_2 = - \frac{2902.39}{T} + 6.498 - .02379 T$$

FIGURE 15
TITRATION OF 200 ml OF A SODIUM PHOSPHATE SOLUTION
(250 ppm PO_4 , $\text{NO}_3/\text{PO}_4 = 2.6$) WITH 0.210 N HNO_3

(The equations for F_1 and F_2 were obtained from References (11) and (12) respectively).

(2) adding the material balance equation:

$$T_3 = [H_2CO_3] + [HCO_3^-] + [CO_3^{=}]$$

(3) changing the electrical neutrality equation to:

$$[Na^+] + [H^+] = [OH^-] + [H_2PO_4^-] + 2[HPO_4^{=}] + 3[PO_4^{\equiv}] + [HCO_3^-] + 2[CO_3^{=}] + [NO_3^-]$$

and (4) changing S in equation (8) to read:

$$S = [Na^+] + [H^+] + [OH^-] + [H_2PO_4^-] + 4[HPO_4^{=}] + 9[PO_4^{\equiv}] + [HCO_3^-] + 4[CO_3^{=}] + [NO_3^-]$$

Changes 1 through 3 give a seventh order polynomial equation for $[OH^-]$.

The calculated results for the acid titration of a 250 ppm PO_4 solution (Na/ PO_4 ratio of 2.6) which contains 2 ppm and 5 ppm CO_2 with 0.210 N HNO_3 are shown on Figure 15. The figure illustrates the phosphate results will be biased on the high side by approximately 2 to 3 ppm PO_4 per ppm carbon dioxide absorbed in the solution.

The effect of other impurities on the titration curve can be calculated in a similar manner.

C. Quality Control of Phosphate Buffer Solution

The composition and pH of the buffer solution (0.025 M Na_2HPO_4 , 0.025 M KH_2PO_4) can be determined by two simple titrations and use of Figure 16 which was calculated using the computer program described in Section VII-B.

The first titration, which determines the molarity of the Na_2HPO_4 in the solution, consists of titrating 50.0 ml of the buffer solution with 0.100 N HCl to a pH of 4.5 ± 0.25 . The molarity of the Na_2HPO_4

is $0.002 V_{\text{HCl}}$ in which V_{HCl} is the ml of 0.001 N HCl required to lower the pH of the solution to 4.5 ± 0.25 .

The second titration, which determines the molarity of the KH_2PO_4 in the solution, consists of titrating 50.0 ml of the buffer solution with 0.100 N NaOH to a pH of 9.2 ± 0.2 . The molarity of the KH_2PO_4 is $0.002 V_{\text{NaOH}}$ in which V_{NaOH} is the ml of 0.001 N NaOH required to raise the pH of the solution to 9.2 ± 0.2 .

The pH of the solution is determined from the molarities of the Na_2HPO_4 and KH_2PO_4 (determined above) using Figure 16.

Data obtained using the above method are shown in Table IV.

Table IV

Determination of Composition and pH of the 0.025M Na_2HPO_4 ,
0.025 M KH_2PO_4 Buffer Solution

Sample	KH_2PO_4 molarity		Na_2HPO_4 molarity		pH at 25C		
	Determined		Determined		From	From	
	By Weighing	Determined By Titration	By Weighing	Determined By Titration	From Weighing Chemicals + Fig. 16	From Titration + Fig. 16	Direct Measurement
1	0.0250	0.0249	0.0250	0.0248	6.86	6.85	6.86
2	0.0250	0.0251	0.0235	0.0231	6.83	6.83	6.85
3	0.0250	0.0251	0.0275	0.0272	6.89	6.88	6.89

Footnote* Data obtained from Messrs. L. Pollack and M. Lew, Mare Island Naval Shipyard, Vallejo, California

D. Determination of Temperature Coefficients for pH and Conductivity

Most pH meters are equipped with temperature compensators which compensate for the change in potential of the electrodes used for the pH measurements. However, the temperature compensators do not compensate for the change in pH of the solution being measured due to the changes in the ionization constants of water and the acid or bases in the solution with temperature. The pH meter manufacturer has no way of knowing what solutions his pH electrodes will be exposed to and therefore has no way of compensating for this change in ionization constants.

VARIATION OF pH AT 25°C WITH
 Na_2CO_3 AND NaHCO_3 MOLARITY

Figure 16

Section VI,A showed how the pH of two buffer solutions change as a function of solution temperature. The pH of phosphate solutions in the phosphate concentration range of 10 ppm to 500 ppm and a Na/PO₄ molar ratio of 2.2 through 3.0 were calculated by the computer program (Section IV). These solutions were shown to have approximately the same changes in pH with temperature over the temperature range of 0 to 50°C. Disodium acid phosphate solutions (Na/PO₄ = 2.0) over the same total phosphate concentration range as above have pH changes with temperature which differ considerably from the changes calculated for the phosphate solutions with Na/PO₄ molar ratios of 2.2 through 3.0. Phosphate solutions with a Na/PO₄ molar ratio of 2.1 have values near the values for the phosphate solutions with Na/PO₄ molar ratios of 2.2 through 3.0. Table V shows corrections for pH which should be applied to pH readings for various phosphate solutions which are made at a temperature other than 25°C in order to obtain the pH value which would have been measured at 25°C.

Table V

Temperature Correction Factors for Sodium Phosphate Solutions
Over the Concentration Range of 10 ppm to 500 ppm and
the Temperature Range 0 to 50°C

Na/PO ₄	Temperature °C										
	0	5	10	15	20	25	30	35	40	45	50
2.0	-0.52	-.40	-.29	-.19	-.09	0.00	+.08	+.16	+.24	+.31	+.37
2.1	-0.90	-.71	-.51	-.33	-.17	0.00	+.15	+.30	+.43	+.55	+.66
2.2-3.0	-0.92	-.72	-.52	-.34	-.17	0.00	+.17	+.31	+.46	+.59	+.72

As shown in Section III, the change in the conductivity of solutions with temperature can be described by the relationship

$$L_t = L_{25} (1 + \alpha (t - 25)) \quad (26)$$

in which

L_t is the conductivity of the solution at temperature t °C,
 L_{25} is the conductivity of the solution at 25°C and
 α is the temperature coefficient (/°C)

The change in conductivity of phosphate solutions over the temperature range 0 to 50°C, the phosphate concentration range of 10 to 500 ppm and the Na/PO₄ molar ratio of 2.0 to 3.0 were calculated using the computer program described in Section IV. The results showed that the temperature coefficient, α , varied from 0.0192 to 0.0236/°C. At a total phosphate concentration of 10 ppm the α values decreased progressively from 0.0219/°C at Na/PO₄ = 2.0 to 0.0192/°C at Na/PO₄ = 3.0 whereas at a total phosphate concentration of 500 ppm, the α values increased progressively from 0.0216/°C at Na/PO₄ = 2.0 to 0.0236/°C at Na/PO₄ = 3.0. A good average value for α over the total phosphate concentration range of 10 to 500 ppm is 0.021/°C or

$$L_t = L_{25} (1 + 0.021 (t - 25)) \quad (27)$$

VIII. Discussion of the Effect of Phosphate Concentration on Solution pH at Various Temperatures

A. Change in pH of Na₂HPO₄ solutions with concentration at 25 and 300°C

Both the computer program and the Reference (9) measured values, given in Figures 2 through 14, show that at 25°C the pH of a phosphate solution of a given Na/PO₄ molar ratio increases and then decreases with increasing concentration. This result was unexpected and the reason for this phenomenon is not known. It has to be connected with the change in the activity coefficients since the activity coefficients are the only variables which change with solution concentration. The computer program does not predict a peak in pH for Na₂HPO₄ solutions heated to 300°C over the concentration range of 1 to 100,000 ppm. Table VI gives values for the pH and activity coefficients over a phosphate concentration range of 1 to 10,000 ppm for phosphate solutions having a Na/PO₄ molar ratio of 2.0. The solutions temperatures are 25°C and 300°C.

Table VI

Changes in the pH and Activity Coefficients for Na₂HPO₄ Solutions Over the Concentration Range of 1 to 10,000 ppm

ppm PO ₄	pH	Temperature 25°C		
		γ_1	γ_2	γ_3
1	8.08	0.994	0.975	0.943
10	8.58	0.980	0.922	0.833
100	9.04	0.940	0.782	0.575
1000	9.33	0.844	0.507	0.217
10000	9.13	0.683	0.218	0.032

<u>Temperature 300°C</u>				
<u>ppm PO₄</u>	<u>pH</u>	<u>γ₁</u>	<u>γ₂</u>	<u>γ₃</u>
1	6.18	0.986	0.945	0.881
10	7.12	0.958	0.842	0.678
100	8.01	0.875	0.585	0.299
1000	8.57	0.674	0.206	0.028
10000	8.74	0.414	0.029	0.0035
100000	8.81	0.25	0.0039	0.0000038

B. Effect of Temperature on Solution pH of Phosphate Solutions with Na/PO₄ Molar Ratios of 2.0, 2.5, and 3.0

Figures 17 through 19 show computer calculated values for pH as a function of temperatures for various sodium phosphate solutions having Na/PO₄ molar ratios of 2.0, 2.5, and 3.0. The pH change for water is shown also on each figure. Since pH is used as a measure of the excess or deficiency of hydronium ions compared to the hydronium ions in pure water, a more revealing figure is shown as Figure 20. This figure is a plot of the solution pH - pH of neutral water versus Na/PO₄ molar ratios. Figure 20 shows that any phosphate solution having a molar ratio greater than approximately 2.0 to 2.1 will decrease in pH relative to neutral water when heated from 25°C to 300°C.

C. Predominant Phosphate Ions at 25°C and 300°C

Figures 21 and 22 show the calculated percentage of the phosphate ions present in 0.1 M sodium phosphate solutions at 25°C and 300°C as a function of solution pH - pH of water. It is noted that heating the solutions has the effect of displacing the pH approximately +2 pH units and that the PO₄⁼ is no longer present in the solutions.

IX. Summary

A method is presented for calculating the pH and conductivity of sodium phosphate solutions. This method, which is developed as a computer program, contains temperature dependent parameters and therefore permits calculation of pH and conductivity values as a function of temperature. Comparison of calculated pH and conductivity values with measured values shows excellent agreement.

Several practical uses of the developed computer program are shown in this paper. These uses are:

FIGURE 18
CHANGE IN pH OF $\text{Na}/\text{PO}_4 = 2.5$ SOLUTION WITH
TEMPERATURE AND CONCENTRATION

FIGURE 17
CHANGE IN pH OF $\text{Na}/\text{PO}_4 = 2$ PHOSPHATE SOLUTIONS
WITH TEMPERATURE AND CONCENTRATION

FIGURE 19
CHANGE IN pH OF PHOSPHATE SOLUTIONS WITH
TEMPERATURE AND CONCENTRATION
 Na/PO_4 MOLAR RATIO = 3.0

FIGURE 20
CHANGE IN pH (RELATIVE TO NEUTRAL WATER)
AS A FUNCTION OF Na/PO₄ MOLAR RATIO

FIGURE 21
PREDOMINANT PHOSPHATE IONS AT 25°C
(9497 ppm TOTAL PHOSPHATE)

FIGURE 22
PREDOMINANT PHOSPHATE IONS AT 300°C
(9497 ppm TOTAL PHOSPHATE)

1. Determination of total phosphate concentration from pH and conductivity measurements.
2. Calculation of acid titration curves and effect of CO₂ absorption on titration curves.
3. Quality control of phosphate buffer solutions.
4. Determination of temperature coefficients for pH and conductivity.

Finally a discussion of the effect of phosphate concentration on solution pH at various temperatures is presented. At 25°C the pH of a phosphate solution for a given Na/PO₄ molar ratio increases and then decreases with increasing concentration. This behavior which is predicted by the computer program is also supported by measured values. At 300°C however, the computer program predicts no peak in pH with increasing phosphate concentration. Also the predominate phosphate ions at 25 and 300°C for 0.1 M phosphate solutions are calculated and presented.

X. References

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Appendix A

Computer Code Abstract

PHOS1

1. Program Name: PHOS1.BAS
2. Computer and Programming Language: BASIC computer language for a DEC-10 computer.
3. Physical Problem Solved: PHOS1 (Ref. 1) calculates the pH and conductivity of sodium phosphate solutions. The equations are applicable for calculation of pH over the temperature range 0 to 300°C; the equations for conductivity are valid over the temperature range of 0 to 50°C. With minor changes to the computer program, titration curves (titrating a particular sodium phosphate solution with an acid) can be obtained.

The effect of carbon dioxide or other impurities on the pH of sodium phosphate solutions can be determined by modifying the program to incorporate the appropriate equilibrium constants, material balance, and electrical neutrality equations and by changing the ionic strength equation to incorporate the presence of the impurity. To determine the effect of carbon dioxide on pH, the above changes result in a seventh order polynomial equation for the hydroxyl ion concentration which is determined by the Newton-Raphson method.

4. Method of Solution: A fifth order polynomial in hydroxyl ion concentration as a function of the ionization constants and the sodium and phosphate concentrations was obtained from the ionic equilibria, material balance, and electrical neutrality equations. The Newton-Raphson method was used to determine the hydroxyl ion concentration. All other ionic concentrations in the sodium phosphate solution were calculated using the hydroxyl ion concentration and the ionic equilibria, and material balance equations.

Uni-, di-, and tri-valent activity coefficients were calculated using the Debye-Huckel theory relating activity coefficients to ionic size, charge, and ionic concentrations. The calculated activity coefficients were compared to an initial assumed value of 1.0 for each activity coefficient. If the calculated activity coefficients differed by more than 0.1 percent from the assumed value of 1.0, the calculated values were substituted into the ionic equilibria equations and new ionic concentrations were calculated. The iteration process was continued until the new calculated activity coefficients and the previously calculated activity coefficients were within 0.1 percent.

pH was calculated from its definition using the above calculated hydrogen ion concentration and uni-valent coefficient. Literature values for the ionization constants, the dielectric constant, the viscosity, and density of water as functions of temperature were used in the computer program to permit pH values to be calculated over a temperature range of 0 to 300°C.

Literature determined values for the ionic conductivity of ions at infinite dilution as a function of temperature over the range 0 to 50°C along with the Onsager-Fuoss equation were used to calculate the conductivity of the phosphate solutions. The Onsager-Fuoss equation relates the ionic conductivity at a given concentration to the ionic conductivity at infinite dilution and the ionic strength of the solution.

By making minor changes to the program, titration curves (titrating a particular sodium phosphate solution with an acid) can be obtained. The required changes consist of: (1) specifying a volume of solution to be titrated, (2) specifying a normality for the acid titer, (3) FOR and NEXT statements to permit definite amounts of acid to be added to the solutions titrated, (4) statements accounting for the dilution of the sodium and total phosphate concentrations after each acid addition, and (5) changing the ionic strength of the solution with each acid addition to account for the acid anion concentration added.

5. Restrictions on the Complexity of the Problem: None.
6. Related and Auxiliary Programs: This program does not supersede nor is it an extension of earlier programs. Other programs are not contained within this program.
7. Typical running time: 2 to 4 seconds.
8. Unusual Features of the Program: see Item 3 above.
9. Status: Production.
10. Machine Requirements: No hardware components, other than a PDP-10, are required for full utilization of the program.
11. Operating System or Monitor: The program requires no deviations from the "standard" operating system.
12. Other Programming Restrictions or Operating Information: No additional information is necessary for the reader to decide the extent of

modifications required to permit use of this program in his operating environment, operating system, programming language, and/or computer.

13. Availability: Copies of the computer program may be obtained by domestic users from:

National Energy Software Center
Attention: Mrs. Margaret Butler
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60440

14. References: J. M. Wright and G. E. VonNieda, "pH and Conductivity of Sodium Phosphate Solutions," WAPD-TM-1302, Bettis Atomic Power Laboratory (1979).

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