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Mathematical Modeling with pH of Diluted Hydrochloric Acid at various Concentrations (Molarity) under Standard Condition (25^oC)

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Abstract: *Hydrochloric acid in chemical industries such as oil well acidification steel pickling, food production, ore and calcium chloride processing, to name but a few, is a commonly used chemical product. Consequently, as an entity that demonstrates various activities at various levels of pH, an essential factor that expresses a solution's chemical conditions (acidity/alkalinity) for a broad array of applications. In this context, at standard conditions (25^oC), the pH of hydrochloric acid [pH=-0.434ln (M) +0.0005], R^2=1] was mathematically designed against its molar concentrations (0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45 & 0.50M) with theoretical hydrogen ion concentration algorithms in solution over a web-based software interface. This model can therefore be applied alternatively to the pH determination of standard solution of hydrochloric acid (molarity) at the specified condition.*

Keywords: Hydrochloric acid, pH, molarity, mathematical modeling and, web-based software.

1.0 INTRODUCTION

About the period 800 AD, Hayyan ibn Jabir discovered hydrochloric acid historically through Iron (II) sulfate and rock salt [1], it was labeled acidum salis and salt spirits. Muriatic or hydrochloric acid (HCl) is a distinctively pungent and colorless inorganic chemical compound. It is considered a strong reagent capable of assaulting the skin across a broad set of possible strength due to its complete nature of dissociation entirely in water [2]. It is a hydrogen chloride gas solution which is also a biologically active portion of gastric acid developed in the digestive systems of mammals including humans. [3] It is processed by reacting water with hydrogen chloride and with many precursors in many forms. The processing of hydrochloric acid on a commercial scale is often combined with the synthesis of various chemicals on an industrial level, including the chloralkali reaction that provides hydrogen, hydroxide, and chlorine which is reacted to generate hydrochloric acid**.** It is a significant industrial chemical reagent employed in the manufacturing of polyvinyl chloride with polymers [5], as a descaling component [5], as a nutrition additive, in the manufacturing of gelatin [6], in the manufacture of leather [7] and control of solution pH [8]. High graded hydrochloric acid, which demands industrial purity such as food, pharmaceutical, and water treatment, is employed in regulating the pH of water process flows [9] [10]. This acid is a very active reagent with the nature of complete dissociation in an aqueous system and is used to obtain salts with Cl-anion as chlorides [11] [12]. It is the recommended titrant in calculating the level and strength of bases because of the distinct endpoint with more accurate results. In quantitative analysis, about 20.2 percent azeotropic hydrochloric acid solution serves as the main standard while its specific composition rests on the ambient pressure when prepared[13]. Generally, it is commonly adopted in the digestion of samples for a metallic determination as required in chemical research [14]. The physical characteristics including boiling points, melting points, density, and pH, rely on its aqueous concentration or molarity [15]. They range from ordinary water at low compositions of approximately 0 percent HCl to hydrochloric acid concentrations of over 40 percent [15]. Hydrochloric acid retains a regular azeotropy at 108.6 °C and 20.2 percent HCl as a binary combination of water and HCl [16]. Moreover, four basic-crystallization eutectic points between the crystal forms as HCl•H2O (68% HCl), HCl•2H2O (51% HCl), HCl•3H2O (41% HCl), HCl•6H2O (25% HCl), and ice (0% HCl) exist [16]. Also, there is a eutectic metastatic point within the ice and the crystallization of HCl•3H2O at 24.8 percent [17].

$$\mathrm{OH^- + HCl \longrightarrow H_2O + Cl^-}$$

$$\mathrm{HCl + H_2O \longrightarrow H_3O^+ + Cl^-}$$

The theory of pH was initially proposed at the Carlsberg Laboratory in 1909 by the Danish chemist Søren Peder Lauritz Sørensen and updated into modern pH in 1924 to match the electrochemical cell specifications and calculations [19]. The symbol from the first papers had H as a suffix to the lower case letter p as pH. However, it disputes the precise interpretation of the p in pH, and he did not disclose the rationale for its usage. The manner in which it can be estimated with potential differences according to him is to represent the negative power of 10 as the hydrogen ion concentration. These phrases begin with p in German, Danish, and French as all the languages reported by Sørensen at the Carlsberg Laboratory were French-speaking, the primary language of science publishing. He as well adopted "p" somewhere else with the paper as it stands for "power," Danish potens or German Potenz, meaning "power," or "potential. He could also have arbitrarily marked the sample solution "p" and the reference solution "q"; as they are usually arranged.[19] The pH scale which is always logarithmic reflects the solution's hydrogen ions concentration inversely as the equation measures the approximate molar concentration with the hydrogen ions from the solution to a negative under base 10 logarithm [20].

$$\mathrm{pH} = -\log_{10}(a_{\mathrm{H^+}}) = \log_{10}\left(\frac{1}{a_{\mathrm{H^+}}}\right)$$

At 25^0C pH of a solution less to 7 is acidic, above 7 are basic and solutions at 7 are neutral. A very strong acid retains a pH value that is less than 0, and a strong base, more than 14 [21]. In other words, acid dissolved in water at 25°C with a pH that is lower than 7 and with an alkali more than 7. At a concentration of a mol per dm^3, the solution composed of hydrochloric acid possesses a pH of 0 relative to an alkali solution such as sodium hydroxide with a pH of 14 with the concentration of 1 mol per dm3. Therefore the pH values calculated are usually in the range of 0 to14, as negative pH values above 14 are very feasible. As pH is a mathematical concept, a variation of one pH unit is similar to an exponential variance in the strength of hydrogen ions. Strong bases and acids are compounds with complete dissociation when interacted with water. This implies that under standard conditions, hydrogen ion concentration in the acidic solution is considered to be proportional to the acid concentration. Typically, hydrochloric acid (HCl) with the pH of 2 with 0.01M solution that is equal to -log10 (0.01) and p [OH] of sodium hydroxide at 0.01M as 2 (pH=12). However, for sodium hydroxide solutions at higher low amounts, the control of self-ionization must be factored in [22]. However, deducing the pH of a diluted hydrochloric acid through a standard model will be a significant development for chemists both at the laboratory and industrial scales.

2.0 METHODOLOGY

A web based simulator was exploited in modeling the pH outputs of hydrochloric acid at the range of 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45 and 0.50M concentrations with complete ionization at 25^oC.

3.0 RESULTS AND DISCUSSION

Table 1. Modeled pH values of hydrochloric acid at specified concentrations

Point	Molarity(M)	Ka	pKa	pH	pOH	[OH−] mol/l	[H3O+] mol/l	Ionization (%)
1	0.05	$1 X 10^7$	− 7.00	1.300	12.700	$2.00 X 10^{-13}$	0.05	100
2	0.10	$1 X 10^7$	− 7.00	1.000	13.000	$1.00 X 10^{-13}$	0.10	100
3	0.15	$1 X 10^7$	− 7.00	0.824	13.200	$6.67 X 10^{-14}$	0.15	100
4	0.20	$1 X 10^7$	− 7.00	0.699	13.300	$5.00 X 10^{-14}$	0.20	100
5	0.25	$1 X 10^7$	− 7.00	0.602	13.400	$4.00 X 10^{-14}$	0.25	100
6	0.30	$1 X 10^7$	− 7.00	0.523	13.500	$3.33 X 10^{-14}$	0.30	100
7	0.35	$1 X 10^7$	− 7.00	0.456	13.500	$2.86 X 10^{-14}$	0.35	100
8	0.40	$1 X 10^7$	− 7.00	0.398	13.600	$2.50 X 10^{-14}$	0.40	100
9	0.45	$1 X 10^7$	− 7.00	0.347	13.700	$2.22 X 10^{-14}$	0.45	100
10	0.50	$1 X 10^7$	− 7.00	0.301	13.700	$2.00 X 10^{-14}$	0.50	100

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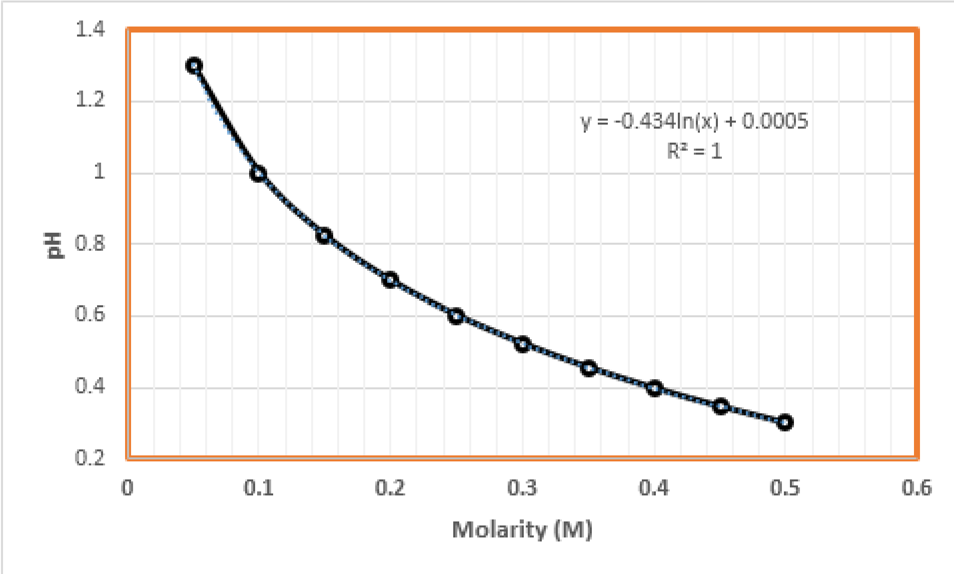

Figure 1. pH – molarity plot of hydrochloric acid.

Table 2. Model Validation

Molarity (M)	pH
0.05	1.300648
0.10	0.999822
0.15	0.823850
0.20	0.698996
0.25	0.602152
0.30	0.523024
0.35	0.456123
0.40	0.398170
0.45	0.347052
0.50	0.301326

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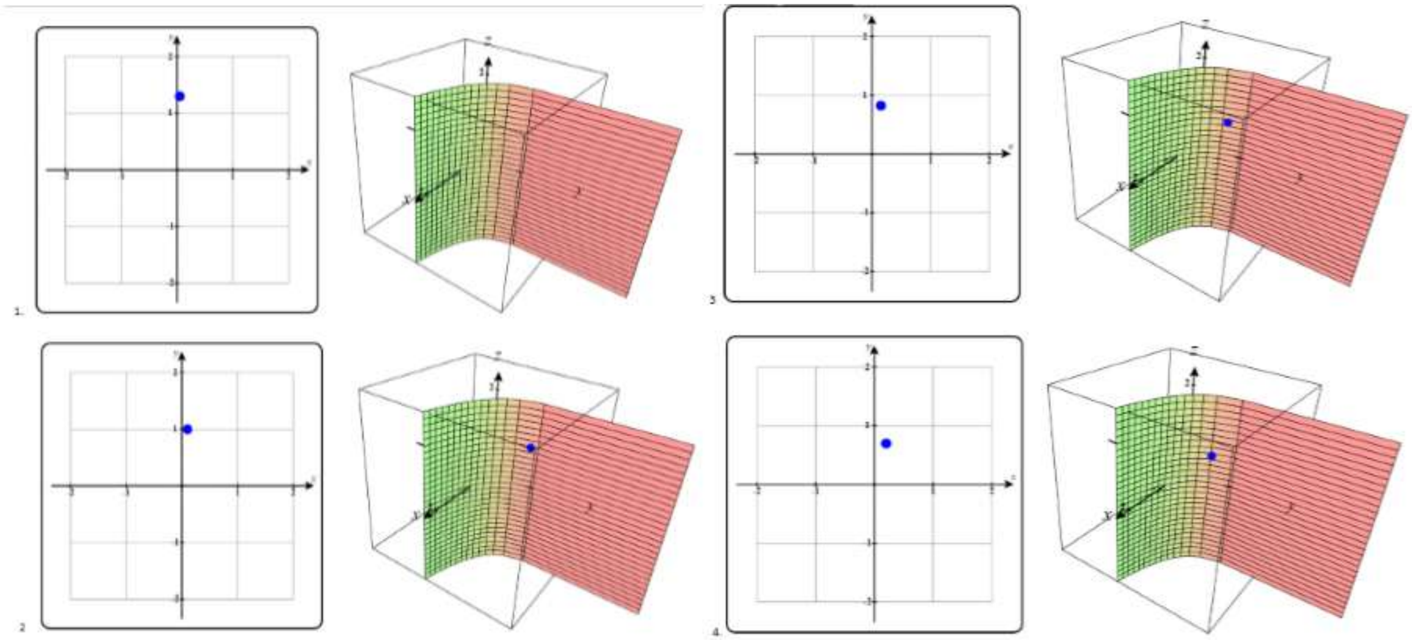


Figure 1. Graphs and 3d plots of points 1, 2, 3 and 4 respectively.

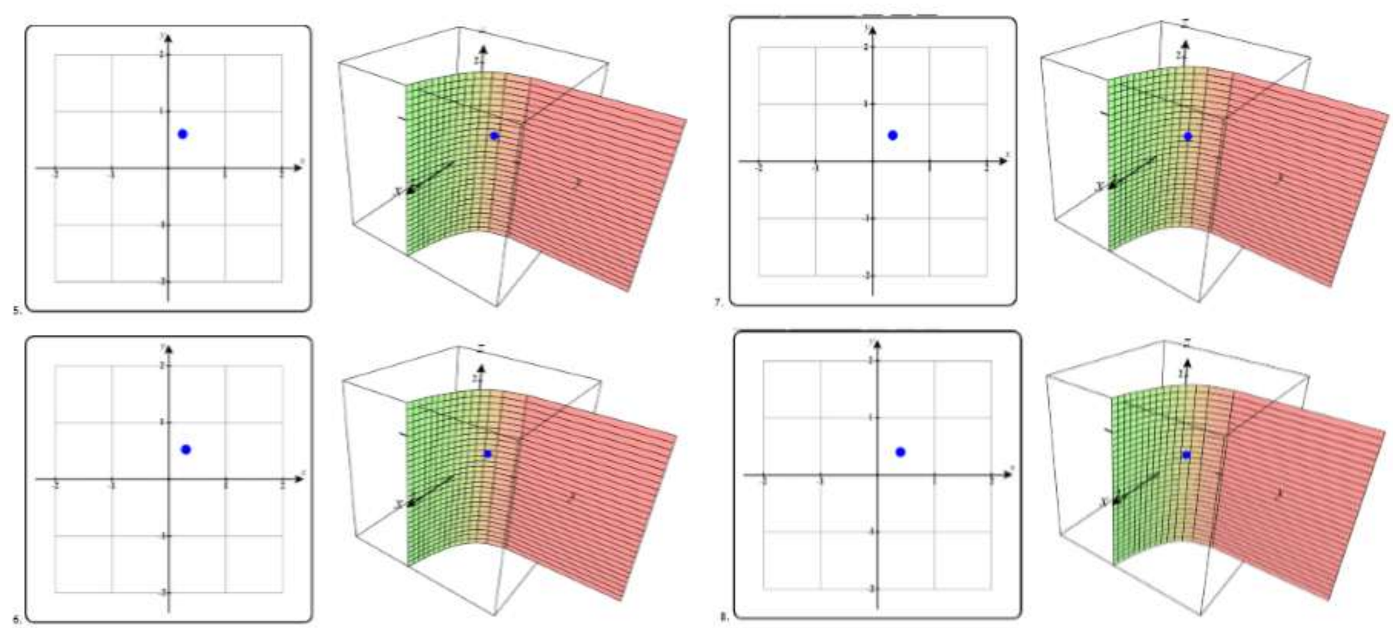
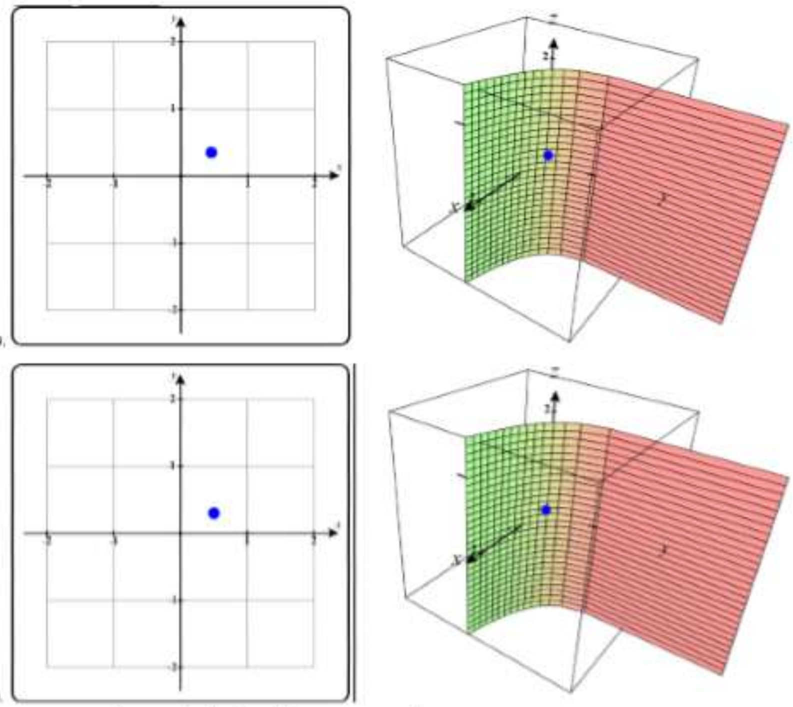


Figure 2. Graphs and 3d plots of points 5, 6, 7 and 8



9.
10.

Figure 3. Graphs and 3d plot of points 9 and 10.

The calculated outcomes from this pH-concentration modeling are disclosed in table 1 and as a plot on figure 1 with the relationship y= -0.434In(x) + 0.0005 at R^2 of 1. Subsequent validation between the two variables (pH and Concentration in molarity) was achieved with the initial values generated by the model. The graphs and the three-dimensional plots presented a visual relationship between the pH and the concentration in molarity through the navigation of the ten coordinates. These declared a logarithmic model and the relationship between the pH and molar concentration of hydrochloric acid.

4.0 CONCLUSION

Chemical industries in general require pH determinations that determine the product quality or monitors chemical reactions. The applications of pH measurements vary widely, from wastewater cleaning, optimizing the texture and flavor of foods and beverages, and enhancing the drying process of dye in the paper and textile sector but a few. Meanwhile, the lifetime of a pH electrode is dependent on the solution conditions which may vary from wastewater, containing a variety of effluents, to pure water in power stations or life science industries. For optimized pH measurements the electrode is required to be calibrated, cleaned, and regenerated at regular intervals. However, this paper has creatively designed a model that can alternatively calculate the pH of a standard hydrochloric acid both in the laboratory and industrial settings.

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