Modeling and Simulation of the Effect of Effluent from Kaduna Refinery and Petrochemical Company on River Kaduna

Uduak George Akpan, Eyitayo Amos Afolabi and Kingsley Okemini

Department of Chemical Engineering, Federal University of Technology Minna, Nigeria

Email: <ugaekon@yahoo.co.uk; elizamos2001@yahoo.com>

Abstract

This study looked at the modeling and simulation of a fundamental model that can be used for predicting the effect of effluent from Kaduna Refinery and Petrochemical Company (KRPC) on River Kaduna using pH as criteria for evaluation. Five model equations were developed using the empirical method of the least squares, and simulated using MathCAD professional software. The simulated results were found to be in a close agreement with the experimental values. The correlation coefficients of 0.9999, 0.9998, 1.0000, 0.9998 and 0.9994 for the distance of 20,40,60 80 and 100m, respectively, from the point of discharge into the water way show that the empirical equations developed are in agreement and perfectly correlated with the experimental results. The model equations developed (using the empirical method of the least squares) can be used to investigate the effect of effluent from Kaduna Refinery and Petrochemicals Company on the quality of river water.

Keywords: Wastewater, pollution, industrial waste, empirical method, MathCAD professional software.

Introduction

Pollution can be defined as the direct or indirect alteration of the physical, chemical, thermal, biological or radioactive properties of any part of the environmental which creates a hazard to health, safety or welfare of any living species. Pollution may occur naturally but mostly occurs due to changes brought by emission of industrial pollutants by careless discharge of industrial and humans' domestic wastewater or sewage and release of excessive heat from industries (Bell 1965; Bolin et al. 1986). Pollution is destructive and capable of causing harm to both living and non living organisms in varying degrees depending on the environment to the extent of rendering it useless to man and hence reducing its benefits. As a matter of fact, apart from a few instances of direct pollution on human beings, it is the pollution through degradation of the environment which occurs in many indirect ways as either solid, liquid or gas affecting the air, land or water (APHA 1965).

Black (1977) described industrialization as a very important tool in every nation's economy and for the improvement of the well being of its citizenry. The negative impact felt by the release of its unwanted byproducts into the environment may be dangerous if allowed to build up and unattended to. While the pollution problem has existed for centuries, the present day industrial (oil) boom and explosion have made it a critical one. The past decade has witnessed a growing concern on the various problems related to environmental pollution and subsequently growing public intervention in the form of public pollution central regulation. From the developed to the developing nations of the world, rich and poor alike, all are concerned and seriously doing something of substance about fighting environmental pollution (White 1987; Klein 1959).

A major serous source of pollution is the industrial effluent discharge by the process industries into the water bodies. Industrial effluent consists of water with varieties of potentially harmful substances which are the sources of environmental pollution. Wastewater is a byproduct of utilized portable water, (domestic wastewater) or industrial process water (industrial wastewater). In the process industries, water could be used as coolant, process water and raw material, etc. It is also used in purification of either the raw materials or finished products. In the process of usage, industrial water becomes polluted and contaminated with various substances it comes in contact with. The discharge of such wastewater or industrial effluents into water bodies such as streams, rivers, lakes, seas, oceans or farmland, etc., could be hazardous to man, aquatic lives, plants and every other living things that derive their water from the polluted sources (Dix 1981; Pontius 1990; James and McDonald 1981).

Considering the importance of water to man, aquatic life and other living creatures, it becomes necessary to develop a mathematical model to evaluate the effects from process industries and the quality of Kaduna River, a tributary of the Niger River which flows for 550 kilometers through Nigeria. А mathematical model of a system only represents the mathematical aspects of a process or system of interest. It gives a basic description of the process and both the physical and chemical phenomena taking place therein. A model describes the physical properties of a system which in real time retains its physical characteristics. Modelling, which serves as the tool of control, becomes important in this study because constant monitoring of the effluents' discharge from the process industries on the river is very necessary. Modelling could eliminate the time and material wastage in carrying out experimental work. Modelling and simulation can be carried out with the aid of the computer using some powerful software packages, like Excel, Polymath, MathCAD, SPSS, and so on. In this study, a mathematical simulation was performed using Excel and MathCAD. The objectives of this study include: the development of model equations that will predict the effect of parameters measured on the pH and BOD of the river Kaduna where effluent is discharged; and also the simulation of the developed equations with MathCAD and Excel together with making comparison between simulated results and the experimental data so as to predict the possible effect of effluent on river Kaduna.

Methodology

Many chemical process developments in the recent years were undertaken through model development. A typical example of a developed model using acidity or alkalinity of a solution (pH) as an optimization criterion was reported in the work of Adeniyi and Odigure (2002). In their work, the pH was modeled using the empirical method of the least squares of the form (Himmelblau 1970; Carnahan *et al.* 1990):

pH = f(Temperature, TSS, COD, Hardness, Ca, Mg, Cl). (1)

This becomes:

 $pH = f(a.T+b.t + c.C_1 + d.H + e.C_2 + f.M + g.C_3).$ (2)

Representing I as the square of error between the observed pH and its predicted value, P:

 $I = (P - f(a.T + b.t + c.C_1 + d.H + e.C_2 + f.M + g.C_3))^2.$ (3)

For *n* experimental values of *P* and other variables:

$$nI = \sum_{n} (P - f(a.T + b.t + c.C_1 + d.H + e.C_2 + f.M + g.C_3))^2.$$
(4)

Adeniyi and Odigure (2002) then concluded that the developed model showed that the pH value is a reflection of the physical, chemical, and technological parameters. They also concluded that the parametric coefficients in the model equation obtained showed the effect of some of the measured parameters on the overall pH value, i.e., increased acidity and alkalinity (Luyben 1990; Odigure and Adeniyi 2002).

Modelling Using the Empirical Method of the Least Squares

The pH of water is a reflection of the resultant effect of Temperature (T), Total Dissolved Solid (TDS), Biochemical Oxygen

Demand (BOD), Sulphate (S), Chloride (Cl), Chemical Oxygen Demand (COD), and Dissolved Oxygen (DO). Therefore,

$$pH = f(T, TDS, BOD, S, Cl, COD, DO), (5)$$

or,

pH = f(a.T + b.TDS + c.BOD + d.S + e.Cl + f.COD + g.DO),(6)

where pH is the dependent variable; a, b, c, d, e, f and g are the coefficients to be determined; and T, TDS, BOD, D, Cl, COD and DO are the independent variables for the desired pH. Since

$$I = (P - pH)^2, \tag{7}$$

on substitution,

 $I = (P - f(a.T + b.TDS + c.BOD + d.S + e.Cl + f.COD + g.DO))^{2}.$ (8)

For n experimental values of P and T, TDS, BOD, S, Cl, COD and DO:

 $nI = \sum_{n}(P - f(a.T + b.\text{TDS} + c.\text{BOD} + d.S + e.\text{Cl} + f.\text{COD} + g.\text{DO}))^{2}.$ (9)

Using MathCAD software to generate different values for the coefficients and then substitute into Eq. (6), one can have:

pH = 0.200.T + 0.019.TDS + 0.0378.BOD - 0.236.S + 0.088.Cl - 0.034.COD + 0.061.DO,

(10)pH = -0.015.T + 0.059.TDS + 0.124.BOD -0.817.S + 0.102.Cl + 3.927x10^{-3.}COD -1.726.DO, (11) pH = 0.0587.T + 0.011.TDS + 7.576x10^{-3.}BOD + 0.014.S - 0.047.Cl + 4.092x10^{-3.}COD -0.051.DO, (12) pH = 0.382.T - 0.021.TDS + 0.190.BOD -1.573.S - 0.019.Cl + 0.051.COD - 1.752.DO, (13) pH = 0.511.T + 0.012.TDS + 0.072.BOD -0.469.S - 0.250.Cl + 0.038.COD - 0.156.DO. (14)

Equations 10, 11, 12, 13 and 14 are modeled equations for samples taken at the distances of 20, 40, 60, 80 and 100m.

Results and Discussion

The data obtained from the experiments and the simulated data are tabulated in Tables 1 to 10. A. comparison of the experimental and simulated pH against run is shown in Figs. 1 to 5.

Run	рН	Т	TDS	BOD	S	CI	COD	DO
1	5.65	30.00	265.00	100.04	8.80	19.70	270.66	9.76
2	5.40	32.00	265.00	110.57	9.01	15.25	290.40	10.97
3	5.87	33.00	267.00	90.47	10.74	20.24	260.01	9.55
4	6.50	28.90	304.40	184.00	18.57	18.45	283.55	10.07
5	6.90	28.00	252.00	192.03	18.70	20.45	254.42	11.78
6	6.20	29.30	268.02	178.80	18.40	18.65	275.21	12.52
7	5.60	32.00	260.00	104.36	9.20	16.75	280.45	12.56

Table 1. Experimental results at the distance of 20m.

Table 2. Simulated results at the distance of 20m.

Dura		T	TDO		0			
Run	рН	1	TDS	BOD	S	CI	COD	DO
1	5.87	30.00	265.00	100.04	8.80	19.70	270.66	9.76
2	5.63	32.00	265.00	110.57	9.01	15.25	290.40	10.97
3	6.08	33.00	267.00	90.47	10.74	20.24	260.01	9.55
4	6.73	28.90	304.40	184.00	18.57	18.45	283.55	10.07
5	7.10	28.00	252.00	192.03	18.70	20.45	254.42	11.78
6	6.42	29.30	268.02	178.80	18.40	18.65	275.21	12.52
7	5.82	32.00	260.00	104.36	9.20	16.75	280.45	12.56

Run	pН	Т	TDS	BOD	S	CI	COD	DO
1	5.89	31.50	286.00	98.78	10.95	20.55	285.01	9.88
2	5.77	31.00	280.00	104.30	9.07	17.86	187.01	10.88
3	5.89	31.50	284.00	101.43	9.01	19.86	254.51	10.81
4	5.90	27.70	275.60	156.00	18.09	17.32	300.10	10.12
5	6.80	28,10	256.05	188.25	17.60	19.87	268.46	11.55
6	5.80	28.40	253.60	196.32	18.75	19.00	261.55	12.01
7	6.20	31.00	280.00	100.23	9.07	21.64	290.34	10.57

Table 3. Experimental results at the distance of 40m.

Table 4. Simulated results at the distance of 40m.

Run	рΗ	Т	TDS	BOD	S	CI	COD	DO
1	5.87	31.50	286.00	98.78	10.95	20.55	285.01	9.88
2	5.75	31.00	280.00	104.30	9.07	17.86	287.01	10.88
3	5.87	31.50	284.00	101.43	9.01	19.86	254.51	10.81
4	5.89	27.70	275.60	156.00	18.09	17.32	300.10	10.12
5	6.79	28.10	256.05	188.25	17.60	19.87	268.46	11.55
6	5.80	28.40	253.60	196.32	18.75	19.00	261.55	12.01
7	6.18	31.00	280.00	100.23	9.07	21.64	290.34	10.57

Table 5. Experimental results at the distance of 60m.

Run	рН	Т	TDS	BOD	S	CI	COD	DO
1	5.80	29.00	302.00	85.54	9.55	16.01	297.54	8.23
2	5.68	29.00	301.00	108.67	8.75	17.90	288.00	11.06
3	5.63	31.50	300.00	106.67	9.85	18.60	238.03	10.05
4	5.60	27.90	276.00	144.00	17.45	18.33	276.05	12.31
5	6.80	28.10	348.25	184.00	17.08	16.55	263.75	10.85
6	6.00	28.00	288.25	184.01	17.80	18.42	270.01	12.66
7	5.70	29.00	300.00	112.08	8.56	154.41	260.90	11.04

Table 6. Simulated results at the distance of 60m.

Run	рН	Т	TDS	BOD	S	CI	COD	DO
1	5.85	29.00	302.00	85.54	9.55	16.01	297.54	8.23
2	5.73	29.00	301.00	108.67	8.75	17.90	288.00	11.06
3	5.68	31.50	300.00	106.67	9.85	18.60	238.03	10.05
4	5.65	27.90	276.00	144.00	17.45	18.33	276.05	12.31
5	6.86	28.10	348.00	184.00	17.08	16.55	263.75	10.85
6	6.05	28.00	288.25	184.01	17.80	18.42	270.01	12.66
7	5.75	29.00	300.00	112.08	8.56	15.41	260.90	11.04

Table 7. Experimental results at the distance of 80m.

Run	pН	Т	TDS	BOD	S	CI	COD	DO
1	6.40	29.00	272.00	113.32	10.01	16.60	260.08	10.01
2	5.26	30.00	278.00	100.55	9.01	16.70	284.09	11.01
3	6.03	31.00	275.00	101.55	10.12	18.75	254.76	9.07
4	5.90	27.90	240.00	158.20	17.82	14.43	283.22	8.99
5	6.50	27.90	300.01	184.00	16.70	18.69	260.02	11.01
6	5.60	28.20	260.40	192.22	18.32	19.23	265.24	11.65
7	6.90	30.00	240.00	107.10	9.00	16.60	270.43	10.86

Run	pН	Т	TDS	BOD	S	CI	COD	DO
1	6.56	29.00	272.00	113.32	10.01	16.60	260.08	10.01
2	5.44	30.00	278.00	100.55	9.01	16.70	284.09	11.01
3	6.19	31.00	275.00	101.55	10.12	18.75	254.76	9.07
4	6.06	27.90	240.00	158.20	17.82	14.43	283.22	8.99
5	6.66	27.90	300.01	184.00	16.70	18.69	260.02	11.01
6	5.76	28.20	260.40	192.22	18.32	19.23	265.24	11.65
7	7.06	30.00	240.00	107.10	9.00	16.60	270.43	10.86

Table 8. Simulated results at the distance of 80m.

Table 9. Experimental results at the distance of 100m.

Run	рΗ	Т	TDS	BOD	S	CI	COD	DO
1	5.30	28.50	240.00	98.54	9.21	15.24	250.77	10.62
2	5.18	28.00	245.00	100.32	8.64	15.14	260.07	10.55
3	6.01	30.00	238.00	98.72	9.65	17.54	235.52	9.65
4	5.60	28.60	244.01	153.01	16.54	17.08	264.21	10.27
5	6.40	27.10	312.00	172.01	16.70	17.08	261.02	10.65
6	6.00	28.00	256.57	184.23	18.21	18.57	259.88	10.94
7	5.80	28.00	210.00	98.67	8.76	11.14	250.86	11.45

Table 10. Simulated results at the distance of 100m.

Run	pН	Т	TDS	BOD	S	CI	COD	DO
1	5.22	28.50	240.00	98.54	9.21	15.24	250.77	10.62
2	5.10	28.00	245.00	100.32	8.65	15.14	260.07	10.55
3	5.94	30.00	238.00	98.72	9.65	17.54	235.32	9.65
4	5.50	28.60	244.01	153.01	16.54	14.65	264.21	10.27
5	6.29	27.10	312.00	172.01	16.70	17.08	261.02	10.65
6	5.89	28.00	256.57	184.23	18.21	18.57	259.88	10.94
7	5.72	28.00	210.00	98.67	8.76	11.14	250.86	11.45

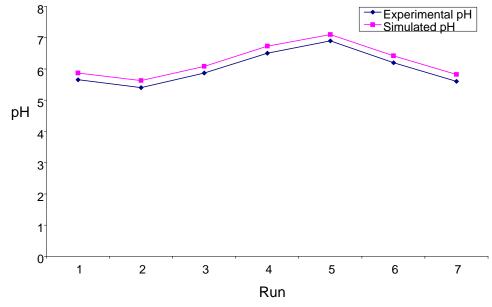


Fig. 1. Plot of Experimental and Simulated pH against Run for 20m.

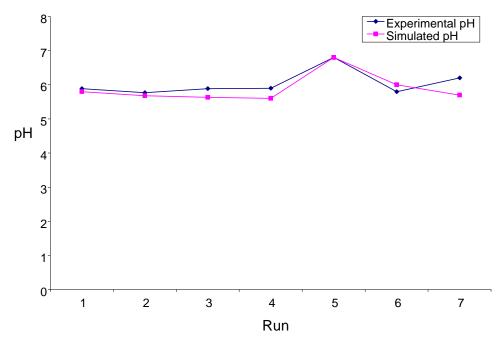


Fig. 2. Plot of Experimental and Simulated pH against Run for 40m.

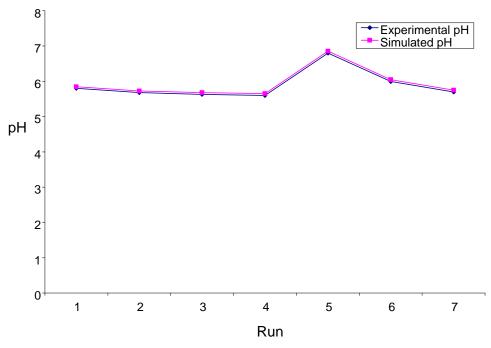


Fig. 3. Plot of Experimental and Simulated pH against Run for 60m.

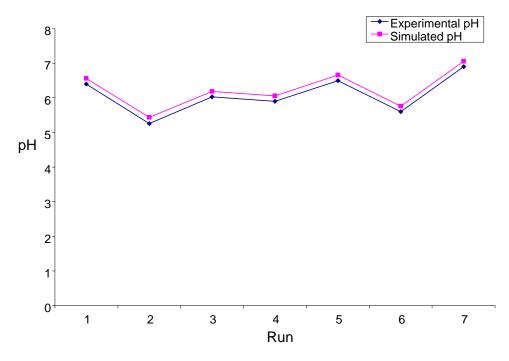


Fig. 4. Plot of Experimental and Simulated pH against Run for 80m.

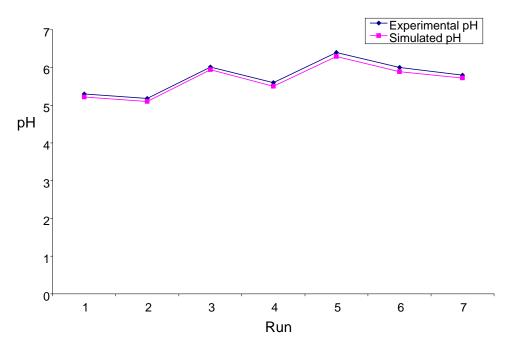


Fig. 5. Plot of Experimental and Simulated pH against Run for 100m.

Discussion

There is a mutual agreement between the model and the experimental results as shown in Figs. 1 to 5. This is based on the closeness of the fitting of the curves to each other. It was observed that there are appreciable rises and falls in the pH of the water in the river into which the effluents are discharged. Generally, the fluctuation trend in the pH was noticed

from all the results, even though the number of turning points of the model is different. From Tables 1 to 10, showing the experimental and the simulated results at different distances, there is a close matching of the experimental results with the simulated ones. Observing the model equations, it can be noticed that some coefficients have positive signs while others have negative signs. The positive sign indicates direct proportionality between the parameters and the pH, while the negative sign indicates inverse proportionality between them. In other words, an increase in any parameters having positive coefficient will lead to an increase in pH, that is, the pH will become more acidic. Conversely, an increase in any of the parameters having negative coefficients will lead to decrease in the pH, hence, the water will become more basic.

One of the measures of testing the validity of an empirical model is the value of the correlation coefficient. The correlation coefficient for different points was calculated with the aid of spreadsheet. From the calculation, the correlations for the modelling at the points of 20,40,60,80 and 100m were found to be 0.9999, 0.9998, 1.0000, 0.9999 and 0.9994, respectively. These good values of correlation coefficients simply indicate the validity of the model equations developed. It can be concluded that the model equations developed have been used to investigate the effect of the effluent from process industries on the water quality of Kaduna River.

The variation between the experimental and simulated results can be attributed to: the non-pattern nature of the experimental data which was due to the meteorological conditions that was not constant throughout the seasons, and the experimental values (which were measures of the concentrations of the river water for the prevailing meteorological condition while the simulated results are the instantaneous values, that is, the concentrations of the river water at any given time).

Conclusion

The correlation coefficients of 0.9999, 0.9998, 1.0000, 0.9998 and 0.9994 for the distances of 20, 40, 60 80 and 100m, respectively, show that the empirical equations developed are in agreement and perfectly correlated with the experimental results. This is because the correlation coefficients tend toward unity. It can be concluded that the model equations developed using the empirical method of the least squares can be used to investigate the effect of effluent from Kaduna Refinery and Petrochemicals Company on the quality of river water.

Recommendation

This work was carried out using Kaduna Refinery and Petrochemicals Company in Kaduna as a case study. It is recommended that industries in other places such as the ones in Lagos and Port Harcourt should be studied and then compared. Also, alternative methods of modelling such as factorial design method of modelling should be used as well.

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