# Model for Computational Analysis of Quantity of Heat Absorbed by Hydrogen Peroxide Solution relative to Weight-Input of Iron Oxide Ore during Leaching

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**Abstract:** Model for computational analysis of heat absorbed by hydrogen peroxide solution (relative to the weight of iron oxide ore added) has been derived. The model;  $Q = e^{1.04(\sqrt{W})}$  was found to be dependent on the weight-input of iron oxide ore. The values of the heat absorbed Q as predicted by the model were found to agree with those obtained from the experiment that the leaching process is endothermic in nature, hence the positive values of the absorbed heat  $Q_{exp}$  and  $Q_M$ . The validity of the model was found to be rooted on the expression  $\ln Q = N(W)^{1/2}$  where both sides of the expression are corresponding almost approximately equal. Maximum deviation of model-predicted quantities of heat absorbed (from the corresponding experimental values) was found to be less than 33% which is quite within the acceptable deviation range of experimental results. [Academia Arena, 2010;2(5):12-14] (ISSN 1553-992X).

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#### 1. Introduction

Nwoye et al.(2009a) derived a model for predicting the initial solution pH at determined final pH and leaching time during leaching of iron oxide ore in hydrogen peroxide solution. It was observed that the validity of the model is rooted in the mathematical expression;  $(\ln t)^{1/2} = N(\beta^C/\alpha^C)$  where both sides of the relationship are approximately equal to 2. The model is expressed as;

$$\beta = \text{Antilog}[0.2439\text{Log}(\alpha^{4.1}(\text{lnt})^{1/2}/3.6)]$$
(1)

The model shows that the initial solution pH is dependent on the values of the final solution pH and leaching time. The respective positive or negative deviation of the model-predicted final pH from its corresponding experimental value was found to be less than 8%, which is quite within the acceptable deviation limit of experimental results depicting the validity of the model.

Model for calculating the solution pH during hydrogen peroxide leaching of iron oxide ore has also been derived by Nwoye et al. (2009b). It was observed that the validity of the model is rooted in the expression  $\ln\gamma = K_C[(\%Fe_2O_3/\%Fe)^N]$  where both sides of the equation are correspondingly approximately equal to 2. The model expressed as;

$$\gamma = \left( \exp K_{\rm C} [(\% F e_2 O_3 / \% F e)^{\rm N}] \right)$$
(2)

The final solution pH was found to depend on the values of the % concentrations of dissolved iron and haematite from experiment. The respective deviation of the model-predicted pH values from the corresponding experimental values was found to be

less than 20% which is quite within the acceptable range of deviation limit of experimental results.

Nwoye (2009) has reported that the heat absorbed by oxalic acid solution during leaching of iron oxide ore can be predicted using the model he derived which works under the process condition; initial pH 6.9, average ore grain size;  $150\mu$ m and leaching temperature;  $30^{\circ}$ C. The model (Nwoye,2009) can be stated as

$$Q = K_{N} \left( \frac{\gamma}{\sqrt[9]{6Fe_2O_3}} \right)$$
(3)

Where

- Q = Quantity of heat absorbed by oxalic acid solution during the leaching process. (J)
- $\gamma$  = Final pH of the leaching solution (at time t).
- %Fe<sub>2</sub>O<sub>3</sub>= Concentration of haematite dissolved in oxalic acid solution during the leaching process.
  - $K_N = 4.57$ (Haematite dissolution constant in oxalic acid solution) determined in the experiment (Nwoye,2008).

Nwoye (2009) carried out further work on the model using the same process conditions and observed that on re-arranging the model as;

$$\% Fe_2O_3 = K_N \left(\frac{\gamma}{Q}\right)$$
(4)

the concentrations of haematite predicted deviated very insignificantly from the corresponding experimental values. In this case, the value of Q was calculated by considering the specific heat capacity of oxalic acid. Values of heat absorbed by the oxalic acid solution during the leaching of iron oxide ore as predicted by the model (Nwoye, 2009) agree with the experimental values that the leaching process is endothermic. This is because all the predicted values of the heat absorbed by the oxalic acid solution were positive. The model shows that the quantity of heat absorbed by oxalic acid solution during the leaching process is directly proportional to the final pH of the solution and inversely proportional to the concentration of haematite dissolved.

A model has been derived (Nwoye et al.,2009c) for calculating the quantity of heat absorbed by oxalic acid solution during leaching of iron oxide ore has been derived. It was observed that the validity of the model is rooted on the expression  $\ln Q = \gamma^N$  where both sides of the expression are approximately equal to 7. The mode;

$$Q = e^{(\gamma \ 1.02)}$$
 (5)

was found to depend on the value of the final solution pH measured during the experiment. The maximum deviation of the model-predicted Q values from the corresponding experimental values was found to be less than 11% which is quite within the acceptable range of deviation limit of experimental results. The positive values of heat absorbed as obtained from experiment and model agree and show that the leaching process is endothermic in nature.

Model for predictive analysis of the quantity of heat absorbed by oxalic acid solution during leaching of iron oxide ore has been derived (Nwoye et al., 2009d). The model:

$$Q = {}^{(0.987(\sqrt{T}))}$$
(6)

The model was found to depend on the value of the final solution temperature measured during the experiment. It was observed that the validity of the model is rooted in the expression  $(\ln Q)/N = \sqrt{T}$  where both sides of the relationship are correspondingly almost equal. The respective deviation of the model-predicted Q values from the corresponding experimental values was found to be less than 21% which is quite within the acceptable range of deviation limit of experimental results. The positive values of heat absorbed as obtained from experiment and model indicate and agree that the leaching process is endothermic in nature.

The aim of this work is to derive a model for computational analysis of the heat absorbed relative to the weight-input of Itakpe (Nigeria) iron oxide ore during leaching using hydrogen peroxide  $(H_2O_2)$  solution.

## 2. Model

The solid phase (ore) is assumed to be stationary, contains the un-leached iron remaining in the ore. Hydrogen ions from the hydrogen peroxide attack the ore within the liquid phase in the presence of oxygen.

## **2.1 Model Formulation**

Experimental data obtained form research work (Nwoye, 2007) carried out at SynchroWell Research Laboratory, Enugu were used for this work.

Results of the experiment as presented in report (Nwoye, 2007) and shown in Table 1 indicate that;

$$\ln Q = N(W)^{1/2}$$
 (approximately) (7)

Therefore

$$Q = e^{N(\sqrt{W})} \tag{8}$$

Introducing the value of N into equation (8)  $Q = e^{1.04(\sqrt{W})}$ (9)

where

- Q= Quantity of heat energy absorbed by hydrogen peroxide solution during the leaching process (J)
- N= 1.04(Weight-input coefficient) determined in the experiment.(Nwoye, 2007)

W = Weight of iron oxide ore used (g) Equation (9) is the derived model.

Table1: Variation of quantity of heat absorbed by  $H_2O_2$  solution with weight of iron oxide ore used.

W(g)	N(√W)	Q (J)	lnQ
18	4.4123	121.68	4.8014
20	4.6510	148.20	4.9986
22	4.8780	171.60	5.1452
26	5.3030	182.52	5.2069
28	5.5032	208.32	5.3391
30	5.6963	226.20	5.4214

## **3. Boundary and Initial Condition**

Consider iron ore in cylindrical flask 30cm high containing leaching solution of hydrogen peroxide. The leaching solution is stationary i.e (non-flowing). The flask is assumed to be initially free of attach bacteria. Initially, atmospheric levels of oxygen are assumed. Varying weights (18-30g) of iron oxide ore were used as outlined in Table 1. The initial pH of leaching solution; 7.34 and leaching time; 30 minutes were used. A constant leaching temperature of 25°C was used. Ore grain size; 150µm, volume of leaching solution; 0.1 litre and hydrogen peroxide concentration; 0.28mol/litre were used. These and other process conditions are as stated in the experimental technique (Nwoye, 2007).

The boundary conditions are: atmospheric levels of oxygen (since the cylinder was open at the top) at the top and bottom of the ore particles in the liquid and gas phases respectively. At the bottom of the particles, a zero gradient for the liquid scalar are assumed and also for the gas phase at the top of the particles. The leaching solution is stationary. The sides of the particles are taken to be symmetries.

#### 4. Model Validation

The formulated model was validated by direct analysis and comparism of Q values from model data and those from the experimental data for equality or near equality.

Analysis and comparism between these data reveal deviations of model data from experimental data. This is believed to be due to the fact that the surface properties of the ore and the physiochemical interactions between the ore and leaching solution which played vital roles during leaching process (Nwoye, 2007) were not considered during the model formulation. This necessitated the introduction of correction factor, to bring the model data to that of the experimental values. (See Table 2)

Deviation (Dv) of model Q values from experimental Q values is given by  $Dv = (Dp - DE) \times 100$  (10)

$$Dv = \left(\frac{Dp - DE}{DE}\right) x \ 100 \tag{1}$$

Where Dp = Predicted data from modelDE = Experimental data

Correction factor (Cf) is the negative of the deviation i.e

$$Cf = -Dv \tag{11}$$

Therefore  

$$Cf = -100 \left( \frac{Dp - DE}{DE} \right)$$
(12)

Introduction of the corresponding values of Cf from equation (12) into the model gives exactly the corresponding experimental Q values. (Nwoye, 2007)

## 5. Results and Discussion

The derived model is equation (9). A comparison of the values of Q from the experimental data and those from the model shows a maximum deviation of 32.23% (Table 2). This is believed to be within a considerable experimental result variation range.

Table 2: Comparison between quantities of heat absorbed as predicted by model and as obtained from experiment.

Q <sub>exp</sub> (J)	$Q_M$ (J)	Dv (%)	Cf (%)
121.68	82.46	-32.23	+32.23
148.20	104.69	-29.36	+29.36
171.60	131.37	-23.44	+23.44
182.52	200.93	+10.09	-10.09
208.32	245.47	+17.83	-17.83
226.20	297.77	+31.64	-31.64

where 
$$Q_{exp} = Q$$
 values from experiment (Nwoye, 2007)

 $Q_M = Q$  values predicted by model.

 $Q_{exp}$  and  $Q_M$  show that the leaching process is endothermic in nature, hence the positive values of Q and heat absorbed during the process.

#### 6. Conclusion

The model was used to evaluate the quantity of heat absorbed by the leaching solution of  $H_2O_2$  during leaching of Itakpe iron oxide ore. It was observed from Q values predicted by the model and those obtained from experiment (Nwoye, 2007) that leaching of the iron oxide ore using  $H_2O_2$  is an endothermic process, hence the positive values of Q from both model and experiment indicating absorbed heat.

Further works should incorporate more process parameters into the model with the aim of reducing the deviations of the model data from that of the experimental.

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