Model for Calculating the Concentration of Upgraded Iron Designated for Production of Stainless Steel Based Biomedical Devices Used in Orthopaedics

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Abstract: Successful attempt has been made to derive a model for calculating the concentration of upgraded iron designated for production of stainless steel based biomedical devices used in orthopaedics. The iron component of the iron oxide ore was upgraded during the pyrobeneficiation of the ore using powdered potassium chlorate. The model-predicted %Fe upgrades were found to agree with a direct relationship between %Fe values and weight-input of $KClO_3$ as exhibited by %Fe upgrades obtained from the experiment. It was found that the model; $\%Fe = \gamma[(\ln(T/\beta))^{2.1277}]$ is dependent on the weight-inputs of $KClO_3$, iron oxide ore and the treatment temperature. The validity of the model is rooted in the expression $(\%Fe/\gamma)^N = \ln(T/\beta)$ where both sides of the expression are correspondingly approximately equal to 3. The maximum deviation of the model-predicted values of %Fe from those of the corresponding experimental values was found to be less than 21% which is quite within the range of acceptable deviation limit of experimental results.
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1. Introduction

Biomaterials such as metals are widely used due to their strength and toughness. While the widely used implant metals (stainless steel, titanium and cobalt alloys) are generally biocompatible, some people are allergic to ions released from these metals. The major problem with metals is the generation of fine wear particles in service that can lead to inflammation and implant loosening [1].

Biometals and associated biomedical devices are used in some parts of the human body. Therefore biocompatibility is expected to prevail in the biometal-biomedical device interaction within the body system. Medical practice has shown that placing a prosthetic device into the body, goes with two considerations which include: functional performance & biocompatibilty and nature of the physiological environment [2].

Functional performance considers the effect of the physiological environment on the biometal/device [2]. This implies that the biometal must satisfy its design requirements with respect to the environment where it serves with time. The varied functions of biometal include: control of blood and fluid flow; eg artificial heart, electrical stimuli; eg pacemaker, light transmission; eg implanted lenses and sound transmission; eg cochlear implant. The material is not expected to degrade in its properties within the environment of the body and must not cause any adverse reactions within the host body. This is in line with the requirement and expectation for biocompatibility [2].

The physiological environment on which biometals and associated biodevices can operate favourably is made up of 0.9M NaCl aqueous solution containing organic acids, proteins, enzymes, biological macromolecules, electrolytes and dissolved oxygen, nitrogen compounds, and soluble carbonate [2]. It was found [2] that pH ≈ 7.4 is normal for physiological extracellular fluid. It has been discovered that cells (eg. inflammatory cells and fibrotic cells) secrete several complex compounds that may significantly affect an implanted biomaterial. Applications of these biometals/devices have been found [3] to be also dependent on mechanical environment: static, dynamic, stress, strain and friction which degrades the metal through corrosion, dissolution and leaching. Medical practice has shown that the resultant degradation affects the materials adversely in terms of strength, fracture toughness and wear resistance [3].

It has been found [4] that pure Ti is useful for dental implants. Ti-6Al-4V has also been found [4] to be useful for investment cast hip and knee implants, dental implants and pacemaker housings due to its mechanical properties (ultimate tensile strength; 825Mpa, elongation; 8%). Ti alloy has also been discovered [4] to have coherent stable passive layer which offers excellent corrosion resistance. They are also resistance to stress corrosion cracking and corrosion fatigue in body fluids. These alloys were also found [4] to permit bone growth at the interface .However, titanium has unsatisfactory wear resistance and may produce wear debris.

Cobalt alloys have been found [5] to possess superior mechanical properties (ultimate tensile strength; 720-890Mpa, elongation; 5-17%) and chemical properties due to finer grain sizes and a more homogenous microstructure. They show excellent wear resistance and have coherent stable passivation layer which gives excellent corrosion resistance.

Steel has been found [6] to be chiefly made up of over 95% Fe and carbon less than 1%. Increasing addition of Cr into the Fe and C matrix and structure re-designs the steel to stainless steel. Addition of nickel to the stainless steel microstructure causes the austenite structure to be maintained at room temperature hence producing austenitic stainless steel [7]. It has been found [7] that 316 stainless steel finds application in early hip implants due to its good strength, ability to work harden and pitting corrosion resistance. The mechanical properties of stainless steel includes: ultimate tensile strength; 190-690Mpa and elongation; 12-40% [7]. Stainless steel usage in biomedical engineering is restricted to temporary device such as screws, plates, fittings and wires for orthopaedics due to potential long term release of Ni^{2+}, Cr^{3+}, and Cr^{6+} into the body [7].

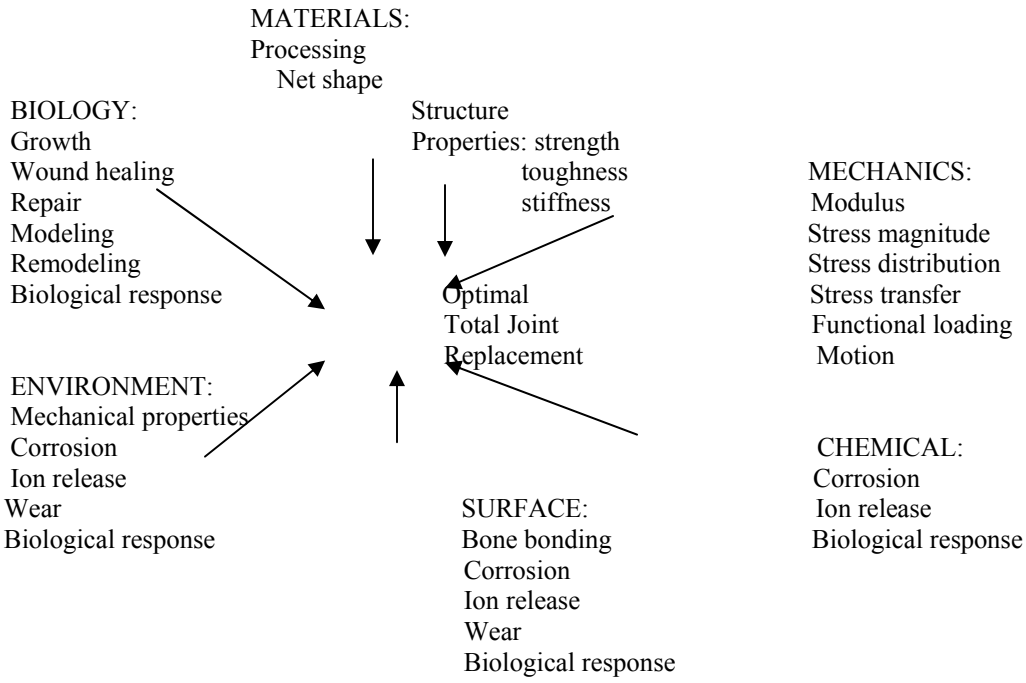

Fig. 1 Joint Replacement Design [5]

Metals dominate the bulk of the implant structure. Co-based alloys are specifically ideal for joint construction because of its high tensile strength, excellent corrosion resistance and excellent fatigue strength [5].

Iron oxide ore from Agbaja (Nigeria) being a primary raw material for the production of Fe used for making stainless steel (used as biomedical device) was found to contain 45.6%Fe and principally goethite, with minor hematite, maghemite, siderite, kaolinite and guartz [8].

An intensive and selective oil agglomeration of the iron ore has been carried out [9]. The researcher, starting from the crude ore Fe content (45.6%), concentrated (upgraded) the ore by oil agglomeration technique to 90% Fe

recovery and 65% Fe assay. He stated that the ore require grinding to minus 5μm to effect adequate liberation. These results were obtained at optimum pH 9. Successful studies on the effect of temperature on magnetizing reduction of Agbaja iron ore have been carried out [10]. The results of the investigation showed that the fine-grained oolitic Agbaja iron ore, which is not responsive to conventional processing techniques, can be upgraded by the magnetizing reduction method with an Fe recovery of 87.3% and Fe assay of 60% at 600^0C.

Attempt has been made to upgrade concentrate Fe recovery [11]. The researchers stated that concentrate Fe recovery decreases progressively below pH 8. In this pH region, oleate used is present as dispersion of oleic acid, and its adsorption on the surface of the iron oxides is similar to the process of hetero-coagulation involving positively charged iron oxide particles and negatively charged oleic acid droplet.

The aim of this work is to derive a model for calculating the concentration of upgraded iron designated for production of stainless steel based biomedical devices used in orthopaedics. The upgrading process stems on the pyro-beneficiation of Agbaja (Nigerian) iron oxide ore using powdered potassium chlorate as oxidant.

2. Model

The solid phase (ore) is assumed to be stationary, contains some unreduced iron remaining in the ore. It was found [12] that oxygen gas from the decomposition of $KClO_3$ attacked the ore in a gas-solid reaction, hence removing (through oxidation) the sulphur present in the ore in the form of SO_2. Equations (1) and (2) show this.

$$2KClO_{3\,(s)} \longrightarrow 2KCl_{\,(s)} + 3O_{2\,(g)} \quad (1)$$

$$S_{(s)}\ \text{Heat} \longrightarrow S_{(g)} + O_{2\,(g)} \longrightarrow SO_{2\,(g)} \quad (2)$$

Nwoye [12] posited that when sulphur inherent in the iron ore is removed in this stance; the concentration of iron present in the ore is upgraded since sulphur is an impurity element.

2.1 Model Formulation

Experimental data obtained from studies [13] carried out at SynchroWell Research Laboratory, Enugu were used for this work.

Results of the experiment as presented in report [13] and used for the model formulation are as shown in Table 1. Computational analysis of these experimental results [13] shown in Table 1, gave rise to Table 2 which indicate that;

$$(\%Fe/\gamma)^N = \ln(T/\beta) \quad \text{(approximately)} \quad (3)$$

Introducing the values of N and β into equation (3);

$$(\%Fe/\gamma)^{0.47} = \ln(T/\beta) \quad (4)$$

Since the inverse of 2.1277 = 0.47

$$(\%Fe/\gamma)^{1/2.1277} = \ln(T/\beta) \quad (5)$$

Multiplying the indices of both sides by 2.1277;

$$\%Fe/\gamma = (\ln(T/\beta))^{2.1277} \quad (6)$$

$$\%Fe = \gamma\,[(\ln(T/\beta))^{2.1277}] \quad (7)$$

Introducing the values of T and β into equation (7) reduces it to;

$$\%Fe = 7.8837\gamma \quad (8)$$

Where

%Fe = Upgraded concentration of iron during the beneficiation process

N= 0.47 (Decomposition coefficient of $KClO_3$ during the beneficiation process) determined in the experiment [13]

(β) =Weight of iron oxide ore added during the beneficiation process (g).

(γ) = Weight of $KClO_3$ added during the beneficiation process (g)

T =Treatment temperature (^{0}C)

N_e =2.1277(Assumed Temperature-Ore Interaction Factor)

I_e = 7.8837(Assumed Iron Enhancement Factor)

Equation (7) or (8) is the derived model**.**

Table 1: Variation of upgraded concentration of iron with weight-input of $KClO_3$ [13]

%Fe	(γ)	(β)
59.71	6	50
62.20	7	50
64.60	8	50
66.40	9	50
67.28	9.5	50
68.50	10	50

Table 2: Variation of $(\%Fe/\gamma)^N$ with ln(T/β)

$(\%Fe/\gamma)^N$	ln(T/β)
2.9445	2.6391
2.7918	2.6391
2.6691	2.6391
2.5581	2.6391
2.5094	2.6391
2.4704	2.6391

3. Boundary and Initial Condition

Consider iron ore (in a furnace) mixed with potassium chlorate (oxidant).The furnace atmosphere is not contaminated i.e (free of unwanted gases and dusts). Initially, atmospheric levels of oxygen are assumed just before the decomposition of $KClO_3$ (due to air in the furnace).Weight of iron oxide ore used; (50g), and treatment time; 360secs. were used. Treatment temperature; 700^{o}C, ore grain size; 150μm, and range of weight of $KClO_3$ used; (6-10g) were also used. These and other process conditions are as stated in the experimental technique [13].

The boundary conditions are: furnace oxygen atmosphere due to decomposition of $KClO_3$ (since the furnace was air-tight closed) at the top and bottom of the ore particles interacting with the gas phase. At the bottom of the particles, a zero gradient for the gas scalar are assumed and also for the gas phase at the top of the particles. The reduced iron is stationary. The sides of the particles are taken to be symmetries.

4. Model Validation

The formulated model was validated by direct analysis and comparison of %Fe values predicted by the model and those obtained from the experiment for equality or near equality.

Analysis and comparison between these %Fe values reveal deviations of model-predicted %Fe values from those of the experiment. This is attributed to the fact that the surface properties of the ore and the physiochemical interactions between the ore and the oxidant (under the influence of the treatment temperature) which were found to have played vital roles during the oxidation-beneficiation process [13] were not considered during the model formulation. This necessitated the introduction of correction factor, to bring the model-predicted %Fe values to those of the experimental %Fe values (Table 3).

Deviation (Dv) (%) of model-predicted %Fe values from experimental %Fe values is given by

$$Dv = \frac{Dm - De}{De} \times 100 \quad (9)$$

Where Dm = Predicted %Fe values from model
De = Experimental %Fe values

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

$$Cr = -Dv \quad (10)$$

Therefore

$$Cr = -\left(\frac{Dm - De}{De}\right) \times 100 \quad (11)$$

Substitution of the values of Cr calculated from equation (11) into the model (equation (7) or (8)) gives exactly the corresponding experimental %Fe values [13].

5. Results and Discussion

The derived model is equation (7) or (8). A comparison of the values of %Fe from the experiment and those from the model shows maximum deviation of the model-predicted values (from experimental values) less than 21% which is quite within the acceptable deviation limit of experimental results hence depicting the reliability and validity of the model. This is shown in Table 3. Table 2 also agrees with equation (3) following the values $(\%Fe/\gamma)^N$ and $In(T/\beta)$ evaluated from Table 1 as a result of corresponding computational analysis. The validity of the model is rooted in equation (3) where both sides of the equation are correspondingly approximately equal to 3.

It is believed that since 2.1277 is the index of the expression $\ln(T/\beta)$ (as in equations (6)and (7)), the values of the process parameters; T and β as applied to the beneficiation process are simultaneously affected by the constant 2.1277 towards iron upgrade. The constant is therefore assumed to be the interaction factor between the treatment temperature and the iron oxide ore (Temperature-Ore Interaction Factor N_e since it is common to both T and β mathematically.

Also 7.8837 was obtained following evaluation of the expression; $[(\ln(T/\beta))^{2.1277}]$ (in equation (7)) which consists of input process parameters; T and β . Based on the foregoing, the constant is assumed to be the Iron Enhancement Factor I_e. In addition, the model-predicted %Fe upgrades were found to show a direct relationship with the weight-input of $KClO_3$ (agreeing with %Fe from the experiment as in Table 1) where I_e acts a multiplying constant of proportionality hence contributing to the iron upgrades mathematically.

Table 3: Comparison between %Fe upgrade as predicted by model and as obtained from experiment [13].

$\%Fe_{exp}$	$\%Fe_M$	Dv (%)	Cf (%)
59.71	47.3022	-20.78	+20.78
62.20	55.1859	-11.28	+11.28
64.60	63.0696	-2.37	+2.37
66.40	70.9533	+6.86	-6.86
67.28	74.8952	+11.32	-11.32
68.50	78.8370	+15.09	-15.09

Where

$\%Fe_{exp}$ = %Fe upgrade from experiment [13]
$\%Fe_M$ = %Fe upgrade predicted by model

6. Conclusion

The model calculates the concentration of upgraded-iron designated for production of stainless steel based biomedical devices used in orthopaedics. The maximum deviation of the model-predicted %Fe values from those of the experiment is less than 21% which is quite within the acceptable deviation limit of experimental results. The validity of the model is rooted in equation (3) where both sides of the equation are correspondingly approximately equal to 3.

Further works should incorporate more process parameters into the model with the aim of reducing the deviations of the model-predicted %Fe values from those of the experiment

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