

Characterization and predictive reaction model for cement-sand-kaolin composite for CO₂ sequestration



M. Abdullahi^{a,*}, J.O. Odigure^b, A.S. Kovo^b, A.S. Abdulkareem^b

^a Department of Chemical Engineering, The Federal Polytechnic, Bida, Nigeria

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

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ABSTRACT

The sustainability and sturdiness of cement based composite is increasingly coming to the forefront of infrastructural design, maintenance and as a green material that is environmentally benign. This paper seeks to develop a predictive mathematical global reaction rate model for atmospheric carbon dioxide sequestration in sandcrete composite of cement, mineral kaolin as supplementary aggregate material (SAM), sand and water. Standard experimental techniques and procedures were used. MatCad Professional (R14) software was used to simulate the developed model equation. Results obtained indicate that the overall global reaction rates for CO₂ sequestration was higher in both experimental and simulated for the developed sandcrete-kaolin (S-K) composite (9.064×10^{-6} and 9.532×10^{-6} mol/kg s) at 30 °C compared to the reference kaolin-free sandcrete (S-S) composite (4.058×10^{-7} and 4.056×10^{-7} mol/kg s) at an early stage of setting (9 h). The quantity of carbon dioxide sequestered after 9 h of carbonation ranges between 0.0185–0.0214 kg/m³ for sandcrete-kaolin composite, while for the reference specimen it ranges from 0.0128 to 0.011 kg/m³ at 30–45 °C. The simulated results based on the developed overall global reaction rates compared strongly with the experimental in most of the parameters investigated. The mineralogical compositions and microstructure changes of the carbonated samples characterized using X-ray Diffractometer (XRD), X-ray Fluorescence (XRF), Scanning Electron Microscopy (SEM) and Diffraction Spectrometer (EDS) showed that addition of mineral kaolin to sandcrete enhanced the rate of CO₂ sequestration.

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1. Introduction

Cement-based materials including sandcrete sequester atmospheric carbon dioxide (CO₂) through a process known as carbonation [1]. Carbonation occurs when carbon dioxide reacts with alkalis in the cement-based materials to form a thermodynamically stable metallic carbonates. Carbon dioxide is the most significant anthropogenic greenhouse gas generated [2]. In order to avoid irreversible climate change effects, greenhouse gas emissions must be stabilize and generation reduced within the next decade [3]. There are different methods currently adopted for carbon dioxide sequestration: ocean sequestration (direct discharge of CO₂ into deep seafloor) and geological sequestration, which involves injection of carbon dioxide into geological formations such as coal seams, deep saline aquifers, oil and gas

field [4,5]. These technologies have some limitations which ranged from high cost, poor mechanical strength, environmental impact and limited geological formations. To address these disadvantages, it is desirable to develop new, more resilient and sustainable cement-based materials with potential to sequester anthropogenic carbon dioxide and in addition maintain the physicochemical and mechanical characteristics of the structure. In order to understand the influence of various parameters on the rate of CO₂ sequestration and for the purpose of control and monitoring, there is need to develop a predictive mathematical model for the process.

Various models have been developed on carbonation of cement-based composite especially on concrete. Papadakis et al. [6] developed and put forward a mathematical model for concrete carbonation based on physicochemical processes. The model showed good conformity in reliance to carbonation depth with age, ambient temperature, aggregate-cement ratio, relative humidity and carbon dioxide concentration. Ramezani-pour et al. [7] in their study applied deterministic and stochastic modeling in determining the depth of carbonation in concrete. The

* Corresponding author at: The Federal Polytechnic, Department of Chemical Engineering, P.M.B 55, Bida, Nigeria.

E-mail addresses: tsowagba@yahoo.com, tsowagbababa@gmail.com (M. Abdullahi).

deterministic model was developed based on the findings of accelerated and in-situ tests. Using a normal distribution tool, the researchers observed that the depth of carbonation after 20 years was 29.13 mm. Saetta et al. [8], used two-dimensional finite element model to study the effects of carbonation attack on the corner reinforcing bars of concrete structure. The study showed that at the corners of a concrete structure, the carbonation depth was greater than 40% when compared to the overall concrete structure surface. Loo et al. [9] studied similar experiment on the rate of concrete carbonation utilizing accelerated carbonation test.

Many prediction models for carbonation coefficient were developed to establish the influence of exposure temperature, concentration of carbon dioxide and curing age in concrete. Odigure [10] studied the rate of sandcrete degradation in the presence of gaseous pollutants. The researcher went further to develop a deterministic model based on the mechanism of cement corrosion, to predict the deterioration of sandcrete structures in Nigeria. The model equation derived incorporated the relationship between concentration of pollutants and depth of their penetration. Odigure [11] investigated the carbonization mechanism of sandcrete block, with the objective to develop holistic model for the migration of carbonized cement minerals' hydrates in sandcrete walls. The migration model gave a complex relationship between the effective diffusions and velocity of the pollutants. However, the sequestration potential of sandcrete and sandcrete related material was not fully documented. In addition, the kinetic and mechanism of reactions that make sandcrete an engineering material in relations to carbonation were not been fully investigated, hence the need for this study. Thus, this work focused on developing predictive mathematical global reaction rate model for atmospheric carbon dioxide sequestration in sandcrete composite of cement, mineral kaolin as supplementary aggregate material (SAM), sand and water.

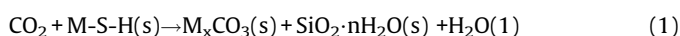
2. Mathematical model

Sandcrete carbonation process is basically a diffusion controlled phenomenon. The rate of diffusion and conversion of carbon dioxide to a stable carbonate strongly depend on the quality and composition of the mix materials [12,6]. Fick's law of diffusion and shell progressive model mechanism were the main principles adopted in developing the proposed overall global reaction rate model of CO₂ sequestration by cement-based sandcrete and sandcrete related product. The carbonation process was assumed to take place in CO₂ atmosphere under isobaric condition, microstructure change was monolayer and carbonation depth increased as reaction progressed with age.

Basic Assumptions

The following assumptions were made to facilitate the derivation of the predictive model equation.

- 1) The particles of sandcrete and calcite formed were completely spherical and relatively equal.
- 2) Surface temperature caused evaporation of moisture to start from the inner core to outer surface of the sandcrete.
- 3) Increase in carbonation decreased the porosity as CO₂ ingress into the sandcrete.
- 4) The major transfer operations were thus based on heat and mass transfer operation.
- 5) The product (solid CaCO₃) of carbonation reaction was retained on the surface of the particles in a monomolecular layer.
- 6) The reaction of metallic mineral hydrates was assumed irreversible;



- 7) Rate of reaction was dependent on temperature, porosity and age.
- 8) Adsorption of CO₂ was by physisorption and chemisorption.
- 9) The sandcrete block was well compacted and therefore available inter-pore spaces were assumed to be spherical.
- 10) Fick's Law holds for diffusion mechanism.
- 11) Diffusion is predominantly in one direction of gas flow except for particles at the edge and Shell progressive model was assumed.
- 12) Sandcrete block lost no material but generates carbonates.
- 13) Rate of dissolution of CO₂ in the pore solution equalled the rate of diffusion into the sandcrete particle.
- 14) Linear isotherm was assumed during the adsorption process.
- 15) Process of Carbonation occurred in stages with soluble alkali hydroxide reacting first followed by other hydrated products (Calcium-silicate-hydrate).

As CO₂ ingress into sandcrete composite and reaction occurred, a layer of CaCO₃ was formed around the unreacted core of cement hydrated minerals [13,14]. This layer must be porous for CO₂ to diffuse in.

η (Effectiveness factor)

$$= \frac{\text{Actual rate for the whole particle}}{\text{Rate evaluated at outer surface conditions}} \quad (2)$$

$$\eta = \frac{r_p}{r_x} \quad (3)$$

$$r_p = \eta r_x \quad (4)$$

It was assumed that the concentration of CO₂ (g) in the atmosphere was proportional to the concentration of CO₂ (aq) in sandcrete block. Adsorption rate equilibrium between the atmospheric CO₂ and the reaction surface was low. Linear isotherm holds for the relationship, which according to [15,1] is given;

$$(C_A)_L = \psi (C_A)_s \quad (5)$$

where $(C_A)_L$ = concentration of CO₂ (aq) in the sandcrete pore solution ($\frac{\text{mols}}{\text{m}^3}$), r_p = global reaction rate (mol/kg. s), $(C_A)_s$ = concentration of CO₂ at the sandcrete particle surface ($\frac{\text{mols}}{\text{m}^3}$), ψ = adsorption equilibrium constant, r_x = intrinsic reaction rate (mol/kg s), $\psi = K_0 e^{-\frac{\Delta H}{RT}}$

K_0 = Adsorption velocity constant for empty surface, monolayer, ΔH = Change in enthalpy per mole of adsorbate as it transfers from gaseous to adsorbed phase (J/mol), R = Gas constant (J/mol K), T = Absolute temperature (K)

Let $\frac{dN_A}{dt}$ be moles of CO₂ adsorbed per unit time per unit particle of sandcrete. The rate law holds for interphase mass transfer from the air to liquid via immobile particles and from liquid to solid.

The rate equations are;

For external diffusion:

$$\frac{dN_A}{dt} = 4\pi r_s^2 K_m [(C_A)_b - (C_A)_s] \quad (6)$$

For diffusion through the sandcrete particle:

$$\frac{dN_A}{dt} = 4\pi r^2 (D_L) e \left[\frac{d(C_A)_L}{dr} \right] \quad (7)$$

For carbonation reaction at the core:

$$\frac{dN_C}{dt} = 4\pi r c^2 K_1 (C_A)_c \quad (8)$$

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