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# Heat flow modeling in the alkaline activation process of fly ash

## Modelamiento del flujo de calor en el proceso de activación alcalina de la ceniza volante

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**ABSTRACT:** Cement production plays an important role in strengthening the infrastructure of growing countries such as Colombia. However, the production of this material has a high energy cost and contributes to the emission of large amounts of $CO_2$. To address these environmental concerns, it is essential to explore alternative materials that can partially or completely replace traditional cement. Alkaline activated cement (AAC) has emerged as a promising candidate in this regard. Due to this, it is necessary to understand the process of alkaline activation and the variables that influence it. This research proposes a phenomenological-based semi-physical model, which predicts the performance of some variables that control alkaline activation: activator concentration (NaOH), heat flow, and degree of reaction. The model results show that with the increment of the activator concentration, the degree of reaction also increases. Furthermore, the model has an accurate response compared with the Freisleben-Hansen model. The integral square error criterion (ISE) was used in this comparison.

**RESUMEN:** La producción de cemento juega un papel importante en el fortalecimiento de la infraestructura de un país en pleno crecimiento como lo es Colombia. Sin embargo, la producción de este material tiene un alto costo energético y contribuye a la emisión de grandes cantidades de $CO_2$. Para abordar estas preocupaciones ambientales, es esencial explorar materiales alternativos que puedan reemplazar parcial o completamente al cemento tradicional. El cemento alcalino activado (AAC) se ha convertido en un candidato prometedor en este sentido. Por ello, es necesario comprender el proceso de activación alcalina y las variables que influyen en él. En esta investigación se propone un modelo semifísico de base fenomenológica, el cual predice el desempeño de algunas variables que controlan la activación alcalina: concentración del activador (NaOH), el flujo de calor y el grado de reacción. Los resultados del modelo indican que con el incremento del activador alcalino (NaOH) el grado de reacción también se incrementa. El modelo presenta resultados precisos comparados con el desempeño del modelo propuesto por Freisleben-Hansen. En esta comparación se utilizó el criterio de error cuadrado integral (ISE).

## 1. Introduction

The production of Ordinary Portland Cement (OPC) has a significant environmental impact, primarily due to its high $CO_2$ emissions and energy consumption. OPC manufacturing is responsible for the emission of large quantities of $CO_2$ ($0.82$ to $1.0 tCO_2/t$ cement ) [1]. This carbon emission is related to the high energy consumption during manufacture: calcination of limestone and the heating of raw materials to temperatures above 1450 °C. [1] Recent studies reported that OPC manufacturing contributes to annual anthropogenic $CO_2$ emissions of approximately 8 and 10% [2]. On the other hand, the energy required for OPC production is as high as 3400 MJ/t

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cement corresponding to 2.5 % of the energy used in the world for the manufacture of materials [3].

Many efforts are being made to reduce the environmental impact of OPC production without requiring significant technological changes. Alkaline activated cement (AAC) has emerged as a promising alternative to OPC. Studies have shown that AAC has better manufacturing and application conditions and can be produced using industrial by-products, thus avoiding waste accumulation [2, 4]. AAC cement only requires approximately 2 MJ/t to be transformed into cement, and it has a carbon footprint for concrete production lower than 9% to that of OPC [3].

One of the scientist's challenges is designing strategies to control and optimize AAC manufacturing processes, including a deep understanding of their kinetic behavior. According to the literature, the correlation between the heat released in the processes of hydration and the maturation of cement can help explain the kinetic behavior of reactions [5]. Some studies have reported models to predict the behavior of the activation process in cementitious materials. Termkhajornkit and Barbarulo proposed a model of the hydration process on OPC [6]. This model included the effect of the temperature on the reaction degree. Moreover, the model offers an understanding of physical and chemical behavior from a phenomenological approach. In a different approach, Parka et. developed an empirical model using artificial neural networks to predict some properties of OPC considering the hydration kinetics [7]. Finally, models based on microcalorimetry experiments [3, 5], phenomenologically based models [8–10] models considering molecular computational approach [11, 12], descriptive based models [13], are some of the most studied models. However, due to the complexity of the phenomena involved, no model accurately represents the dynamics of heat flow associated with alkaline activation in all its stages [4, 14–16].
This research proposes a phenomenological model with a semiempirical base to predict the performance of key variables controlling alkaline activation, such as NaOH concentration (alkaline activator), heat flow, and degree of reaction.

## 2. Methodology

The methodology employed in this study consisted of three stages: theoretical, simulation, and validation. In the theoretical stage, a systematic literature review was carried out to find models that represent the process of alkaline activation and determine the relevant variables and equations required to structure the model. The simulation stage involved solving the mathematical model using commercial software, specifically Matlab®. In accordance with the differential equation to be solved and the recommendations found in [17], the ode45 integration method was used in Matlab ®. Finally, the proposed model was validated at different operating points by comparing the simulation results with other models reported in the literature, particularly with the Freiesleben-Hansen model [18]. The Freiesleben-Hansen model has been widely used to relate the maximum heat generated in a hydration process and activation alkali process and to predict the degree of reaction. With the validation purpose, an integral square-error criterion (ISE) under the Freiesleben-Hansen model and the proposed model was performed. For further information on the integral square error criterion (ISE), additional references can be consulted [19].

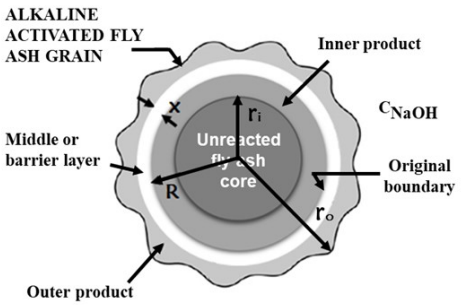



**Figure 1** Shrinking Core Model Schematic Representation. Adapted from [14]

## 3. Model of alkaline activation

In this alkaline activation model, the influence of the activator, properties of fly ash, and curing temperature on the process are considered. It is assumed that alkaline activation will start when fly ash and the activator come into contact, and the product formed by the process adheres spherically to the fly ash particles. As shown in Figure 1, the first layer formed is a thin barrier or intermediate layer (of thickness x), which is composed of a metastable product formed by ions from the dissolution of the process at the stage of the latent period. The barrier layer gradually disappears, which may be because it dissolves or becomes more permeable over time. Additionally, the formation of two different layers of products is considered, the inner product and the outer product. The reaction is followed by the variation of the radius ri of the spherical particle. The above corresponds to Shrinking Core Model: [14, 20].

The Shrinking Core model equation is given by Equation 1, Where ri is the radius of the unreacted fly ash core, $r_0$ is the outside particle radius, R is the initial radius of the fly ash particle, a is the number of moles of the alkaline solution reacting per mole of fly ash consumed,

the parameters $D_x, D_i, D_0$, are the diffusivities through the barrier layer, inner and outer products, respectively, and $\mathrm{C_{NaOH}}$ is the concentration of the alkaline solution (NaOH). In addition, k is the first-order reaction rate constant, $\rho$ is the molar density of fly ash, and x is the thickness of the barrier formed in the latent period.

$$\frac{\mathrm{dr}}{\mathrm{dt}} = \frac{-\mathrm{C_{NaOH}}/\mathrm{a}\rho}{\left[\frac{1}{\mathrm{k}} + \frac{\mathrm{r_i^2}}{\mathrm{D_i}}\left(\frac{1}{\mathrm{r_i}} - \frac{1}{\mathrm{R}}\right)\right] + \frac{\mathrm{xr_i^2}}{\mathrm{D_y R^2}} + \frac{\mathrm{r_i^2}}{\mathrm{D_0}}\left(\frac{1}{\mathrm{R}} - \frac{1}{\mathrm{r_0}}\right)} \quad (1)$$

Reaction / Diffusion In inner product | Diffusion in the barrier layer | Diffusion in outer product.

Equation 1 considers three important phenomena in alkaline activation: reaction/diffusion in inner product, diffusion in the barrier layer, and diffusion in outer product. The disappearance of the barrier layer is given by Equation 2 [20]:

$$x = x_0 e^{-\beta(t-t_0)} \quad (2)$$

Where $x_0$ is the initial thickness of the barrier layer, $\beta$ is the rate constant of the disappearance of the barrier layer and $t_0$ is the time where the barrier layer is formed.
The degree of reaction of alkaline activation can be described by the following Equation 3 [14, 20]:

$$\alpha = 1 - \left(\frac{r_i}{R}\right)^3 \quad (3)$$

Finally, the heat flow accumulated during the alkaline activation process, in which the reactions that occur are exothermic, is given by Equation 4: [14, 20]

$$Q(t) = Q_{\max}\alpha \quad (4)$$

Where $\mathrm{Q_{max}}$, is the maximum heat released in the alkaline activation. In Table 1, the parameter values are shown.
The following assumptions are made:

- i) Fly ash is made up of spherical particles that are uniform in size.
- ii) Sodium hydroxide (NaOH) is considered as the transported (diffusing) reagent during the activation process.
- iii) The density of compounds involved in the process is assumed to remain constant over time and with temperature changes.
- iv) The kinetics of the reactions occurring during alkaline activation are assumed to follow a first-order reaction rate.
- v) The thickness of the metastable barrier layer is modeled as an exponential function basis on references [14] and [20].

## 4. Results and analysis

In order to validate the proposed model, the results were compared with the results from the model by Freisleben-Hansen reported in the literature [3, 5, 18]. Freisleben-Hansn model is highly accurate in fitting the experimental data, which makes it well-suited for comparisons with other models. This is primarily since the parametric adjustment process filters out the inherent variations present in the experimental data resulting from the precision limitations of the equipment used. As a result, it provides a clean curve that can be effectively compared with other models, allowing a more reliable assessment of their performance and predictive capabilities. Figure 2 shows the accumulated heat obtained through the Freiesleben-Hansen and the proposed model. For both models, a NaOH concentration of 10 M and a temperature of 25° are considered. As we can see, the two models present the same dynamic behavior of the accumulated heat during the activation process. The Freiesleben-Hansen model presents more accumulated heat (nearly 13%) than the proposed model. The most significant difference between the models is that the Freiesleben-Hansen model does not consider the first stage of alkaline activation; this is the reason why the Freiesleben-Hansen model begins the activation dynamic with 20 (J/g). In this first stage or initial period, the dissolution and breaking of bonds of the ash components are carried out. The proposed model considers this initial period (Reaction/Diffusion term on Equation 1). Nevertheless, because of the mathematical structure, specifically, due to the model order, the curve of accumulated heat is not similar to that of the experimental data in this stage. Using the integral square-error criterion (ISE) between the two analyzed models, an ISE= 2,040 was obtained [19]. This value indicates that there is a 97.96% similarity in the temporal behavior of the two curves.

In the literature, it is reported that the concentration range of the alkaline activator (NaOH) yielding the best results in alkaline activation is typically between 6 and 10 M [21]. Therefore, the analysis in this study focused on three concentration values within this range: 6 M, 8 M, and 10 M. As shown in Figure 3, an increase in the concentration of NaOH favors alkaline activation. This effect is due to the fundamental role of the alkaline activator since it is responsible for dissolving the aluminosilicate (fly ash) and accelerating the reaction [23]. However, concentrations above 10 M of NaOH lead to system saturation, which is unfavorable for the properties of the cementitious material [21] and thus were not considered in this study.

Upon contact of the fly ash particles with the alkaline activator, heterogeneous exothermic reactions have initiated releasing a certain amount of energy [4].

**Table 1** Model parameters

| Parameter | Meaning | Value | Unit | Data taken from |
|---|---|---|---|---|
| R | Particle size | $15.0*10^{-4}$ | cm | [21] |
| $C_{NaOH}$ | Concentration of the sodium hydroxide | $(6.0-10.0)*10^{-3}$ | $mol/cm^3$ | Experimental data |
| a | Number of moles NaOH reacting per mole of fly ash consumed | 5 | - | Experimental data |
| $\rho$ | Density of fly ash | $9.7*10^{-3}$ | $mol/cm^3$ | [21] |
| $D_x/x_0$* | Ratio of effective diffusivity coefficient of barrier layer and thickness. | $3.4*10^{-7}$ | cm/h | Fitting process |
| $t_0$ | Time where the barrier layer is formed. | 1.0 | h | Experimental data |
| $\beta$ | Rate constant of disappearance of the barrier layer. | 1.4 | - | Experimental data |
| $D_i$ | Effective diffusivity disappearance of the barrier layer. | $8.6*10^{-8}$ | $cm^2/h$ | [11, 20] |
| $D_0$ | Effective diffusivity disappearance of the barrier layer. | $4.2*10^{-7}$ | $cm^2/h$ | [22] |
| k | Kinetic constant at 25°C | $5.4*10^{-5}$ | cm/h | [3] |

*This parameter was found through a fitting process, in which the output variables and the ranges reported in the literature for materials like AAC were considered [20, 22].

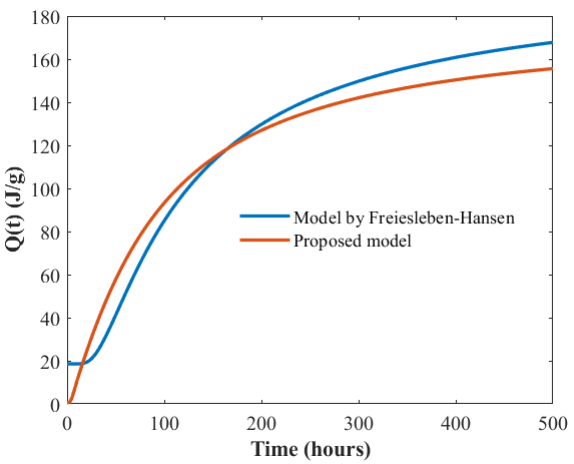



**Figure 2** Comparison of the accumulated heat of the alkaline activation obtained with the proposed model and model by Freiesleben-Hasen

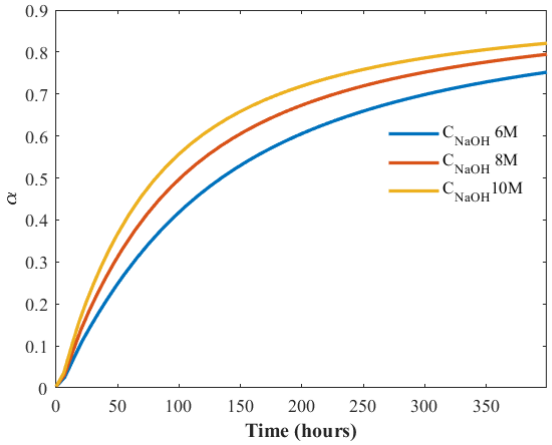
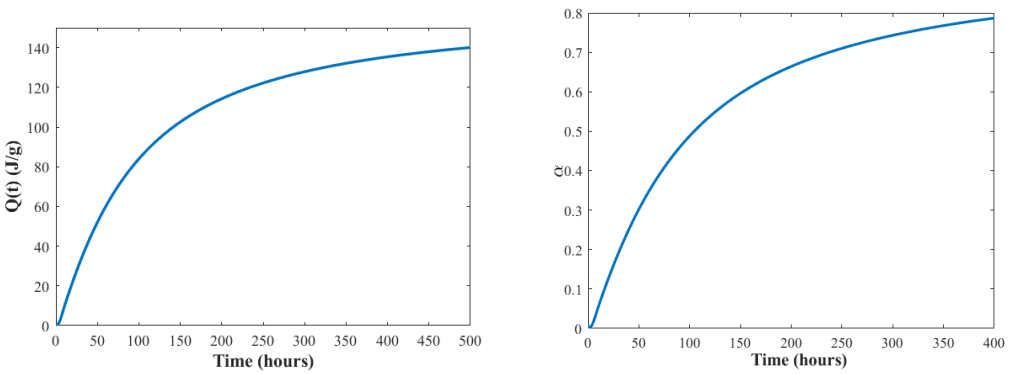



**Figure 3** Effect of activator concentration (NaOH) on the degree of reaction of alkaline activation at $25°C$




**(a)** a **(b)** b

**Figure 4** a) Heat accumulated during the alkaline activation process at $25°C$ and 8M NaOH. b) Degree of reaction of alkaline activation at $25°C$ 8M NaOH

Figure 4a) represents the predicted energy release during the alkaline activation process at $25°C$ with an NaOH concentration of 8 M, reaching a value of 140 J/g after a curing time of 500 hours. Understanding this energy release can help predict the behavior of activated cement in real-world applications, addressing performance issues related to mechanical properties, and even facilitating the design of new cementitious materials [14, 24, 25]. Figure 4 b) shows the evolution of the reactions of the alkaline activation process through the degree of reaction. Particularly, when the curing time was 500 h, a degree of reaction of 0.9 was reached. If we want to improve this degree of reaction, we must analyze factors such as the concentration of the activator (NaOH), the chemical and physical composition of the ash, and the temperature at which the alkaline activation is being given. These factors significantly influence the process and could contribute to optimizing alkaline activation [23].

## 5. Conclusions

In this study, a phenomenological-based semi-physical model was proposed for the alkaline activation of fly ash with sodium hydroxide. The most significant conclusions are summarized below:

In the proposed model, we can see the kinetics variation of fly ash, which accounts for the degree of reaction in the alkaline activation. Additionally, it allows the correlation between the degree of hydration and the heat flow observed during the evolution of the process. Understanding these relationships, makes it possible to assess the concentration of species involved in alkaline activation and identify conditions for process improvement.

Diffusive and reaction processes in a fly ash sphere when contacting NaOH are represented by a phenomenological model (proposed model). Unlike parametric models such as Freisleben-Hansen [3, 21], the proposed model takes into account the initial phase of the process.

This work explores the potential of using a phenomenological model to represent and predict the degree of hydration and heat flow, which constitutes the basis for estimating the evolution of the reaction kinetics on AAC.

## 6. Declaration of competing interest

We declare that we have no significant competing interests, including financial or non-financial, professional, or personal interests interfering with the full and objective presentation of the work described in this manuscript.

## 7. Funding

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## 8. Author contributions

M.E. Adaptation of the model to alkaline activation, analysis of results and drafting of the article. J.S.R. Contributed to the adaptation of the model to alkaline activation, simulation and analysis of results and critical manuscript revision. J.M and A.H.M. were involved in the analysis of results and critical manuscript revision.

## 9. Data availability statement

The authors confirm that the data supporting the findings of this study are available within the article [and/or] its supplementary materials.

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