- Technical Paper -

TOWARDS AMINE-BASED CO_2 CAPTURE IN CEMENT-BASED MATERIALS

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ABSTRACT

CO_2 capture by amines using cement-based materials is vital to reduce the CO_2 in the environment. In this study, three different amines (AEEA, MAE and MDEA) from different amine groups were selected. Moreover, their effects on the precipitation of $CaCO_3$, pH and the type of polymorph of $CaCO_3$ were investigated during carbonation in different Ca-rich solutions ($Ca(OH)_2$, C-S-H and hydrated cement powder). Results indicated that MAE obtained the highest precipitation of $CaCO_3$ in all three Ca-rich solutions. In addition, amine addition influenced the polymorph type of $CaCO_3$.

Keywords: CO_2 capture, amine, cement-based materials, polymorph of $CaCO_3$, Ca-rich solutions.

1. INTRODUCTION

Carbon capture is essential to mitigate global warming as Carbon dioxide (CO_2) is the primary greenhouse gas contributing to global warming [1]. CCUS (carbon capture, utilisation, and storage) is a promising technology in the fight against global warming [3]. CO_2 capture can be achieved by CO_2 mineralisation using alkaline minerals such as steel slag, fly ash and cement wastes, as they can form stable carbonates by reacting with CO_2 [1]. Among those alkaline minerals, using cement-based materials to capture CO_2 is beneficial to the environment and the cement-based material itself as it forms $CaCO_3$ as a carbonated product preferable in cement chemistry to reduce porosity. Even though cement-based materials have the ability to capture CO_2 through mineralisation, the reaction is prolonged. Therefore it is necessary to accelerate the mineralisation by introducing some other techniques.

There are several techniques to capture CO_2 from the environment. Among them, amine-based CO_2 capture by absorption technique is the most mature and efficient technique [4]. Amine is derived from ammonia, where substituents, such as alkyl or aryl groups, have replaced one or more hydrogen atoms. There are three types of amines such as primary, secondary and tertiary, categorised by how many carbon atoms are attached to the nitrogen atom [5]. Moreover, amines can be divided into hindered amines and unhindered amines. Hindered amine concept is based on the reaction rates of the acid gases with different amine molecules [6]. Sterically hindered amines are compounds in which the nitrogen atom of the amine molecule is partially shielded by neighbouring groups so that larger molecules cannot easily approach and react with the nitrogen. In this study, researchers are focusing attention on the formation of bicarbonates as it will give benefits to the cement properties.

Despite the existence of several studies on the incorporation of amine for CO_2 capture in alkaline wastes, such as fly ash, no research has yet been conducted on incorporating amine with fresh cement-based materials for use as a green building material. The capture of CO_2 using cement-based material has the potential to capture a significant amount of CO_2 through the construction of concrete buildings. However, before amines can be directly used with cement paste, mortar, and concrete, it is essential to investigate the reaction mechanism of amine with CO_2 and each Ca-bearing hydrated phase, such as $Ca(OH)_2$ and C-S-H. Therefore, this study aims to identify how each hydrated phase reacts with CO_2 in the presence of amine, what the resulting carbonated products are, and which amine is suitable for capturing more CO_2.

This study investigates the effect of different amines on CO_2 capture and explores their performance in Ca-bearing phases. In this study, 2-(2-aminoethylamino)ethanol (AEEA) from primary and secondary amine, 2-(methylamino)ethanol (MAE) from secondary hindered amine, and *N*-methyldiethanolamine (MDEA) from tertiary amine were selected to compare their ability to capture the CO_2 in Ca-rich media such as $Ca(OH)_2$, C-S-H and hydrated cement powder. Optimum process parameters such as water/powder ratio, carbonation time and amine concentration were selected after conducting the parametric study. The performance of precipitation of $CaCO_3$, pH and the formation of polymorphs of $CaCO_3$ were systematically studied.

The novelty of this research is that it is the first time introducing a revolutionary method for enhancing CO_2 mineralisation in cement-based materials by

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selecting an appropriate amine without significantly affecting cement chemistry. Upon the selection of an appropriate amine, the corresponding amine will undergo testing with cement paste, mortar, and concrete in order to conduct further investigations for potential real-world applications. This unprecedented research paves the way for the successful fixation of CO_2 from the atmosphere in cement-based materials and lays a strong foundation for industrial implementation.

2. PROCESS DESCRIPTION AND CHEMISTRY

2.1 Process Description

Fig.1 shows the concept of CO_2 capture using amines by mineralisation. As shown in Fig.1, Ca-rich solutions with $Ca(OH)_2$ / C-S-H / hydrated cement powder was added to the amine, and then CO_2 was introduced to the resulting solution for a specific time. As a result of carbonation reactions, $CaCO_3$ was precipitated, and a regenerated amine was formed. The degree of CO_2 mineralisation was evaluated by measuring the weight percentage of $CaCO_3$ in the precipitate after carbonation. Furthermore, the pH of the solution was measured to identify the effect of amine on pH.

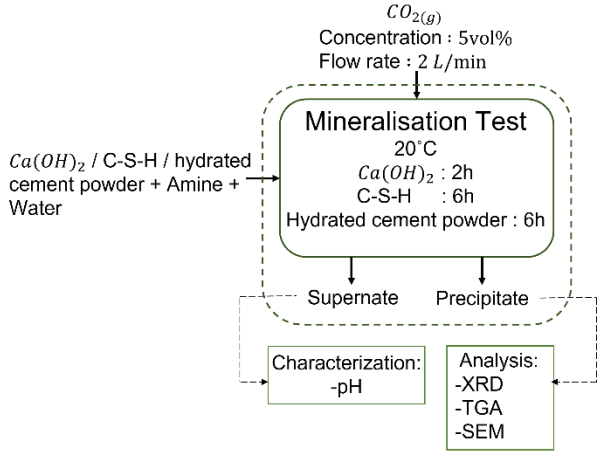
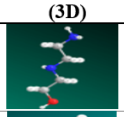
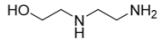
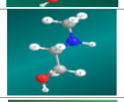
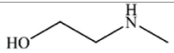
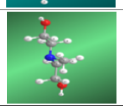
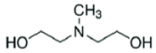


Fig.1 Schematic diagram of the proposed mineralisation process using amine.

2.2 Process Chemistry

Table 1 Chemical properties of amines

Amines	Chemical structure (3D)	Chemical structure	MW (g/mol)	pKa
AEEA			104.15	9.82
MAE			75.11	9.95
MDEA			119.16	8.65

The reaction mechanisms of AEEA, MAE and MDEA with CO_2 and their equilibrium constants have been found in past studies [4,5]. The reaction mechanism involves three stages such as CO_2 absorption, mineralisation, and amine regeneration. Moreover, CO_2 absorption forms two types of products: carbamates and bicarbonates. The Chemical Properties of selected amines are summarised in Table 1.

(1) Reaction chemistry of AEEA

Primary and secondary amines are carbamate-formation amines. AEEA is subjected to carbamate formation reactions as it contains both primary and secondary amine groups [4]. A set of chemical reactions for AEEA can be written as follows [4]:

Physical solubility of CO_2.

$$CO_{2(g)} \rightleftharpoons CO_{2(l)} \quad (1)$$

Ionisation of water.

$$H_2O \rightleftharpoons H^+ + OH^- \quad (2)$$

Formation of carbamate. (CO_2 absorption)
For primary amine in AEEA;

$$CO_2 + 2RNH_2 \rightleftharpoons RNH_3^+ + RNHCOO^- \quad (3)$$

For secondary amine in AEEA;

$$CO_2 + 2R_1R_2NH \rightleftharpoons R_1R_2NH_2^+ + R_1R_2NCOO^- \quad (4)$$

Hydration. (This reaction occurs only at high pressure [7])
For primary amine in AEEA;

$$RNHCOO^- + H_2O \rightleftharpoons RNH_2 + HCO_3^- \quad (5)$$

For secondary amine in AEEA;

$$R_1R_2NCOO^- + H_2O \rightleftharpoons R_1R_2NH + HCO_3^- \quad (6)$$

Dissociation of CO_2.

$$CO_{2(l)} + H_2O \rightleftharpoons H^+ + HCO_3^- \quad (7)$$

Dissociation of bicarbonate ion.

$$HCO_3^- + H_2O \rightleftharpoons CO_3^{2-} + H_3O^+ \quad (8)$$

Carbonation. (Mineralisation)

$$Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3 \downarrow \quad (9)$$

Dissociation of the protonated AEEA. (Amine regeneration)

$$RNH_3^+/R_1R_2NH_2^+ \rightleftharpoons RNH_2/R_1R_2NH+H^+ \quad (10)$$

Where $R, R_1, and\ R_2$ are used for $OHCH_2CH_2NHCH_2CH_2-, OHCH_2CH_2-, and -CH_2CH_2NH_2$, respectively.

(2) Reaction chemistry of MAE

MAE forms bicarbonate during CO_2 absorption as the carbamate ion is unstable for sterically hindered amines due to the neighbouring group's hindrance to the nitrogen atom in the amine group. The reaction mechanism is the same as AEEA except for the further reaction of hydrolysis of carbamate as it is a secondary hindered amine. Only reactions for the primary three steps (CO_2 absorption, mineralisation, and amine regeneration of reaction mechanism) have been

summarised for MAE, as other reactions have already been discussed in the previous section. Chemical reactions for MAE can be written as follows:

CO_2 absorption

$$MAE + CO_{2(l)} + H_2O \rightleftharpoons MAEH^+ + HCO_3^- \quad (11)$$

Mineralisation

$$Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3 \downarrow \quad (12)$$

Amine regeneration

$$MAEH^+ \rightleftharpoons MAE + H^+ \quad (13)$$

(3) Reaction chemistry of MDEA

MDEA forms bicarbonate during CO_2 absorption. Donaldson and Nguyen [8] mentioned that tertiary amine could not form carbamate as there is no hydrogen atom bonded to the nitrogen atom of the amino group. The reaction between CO_2 and the tertiary amine proceeds, as shown below. Here, amine provides an enormous sink for protons produced by slow CO_2 hydrolysis.

CO_2 absorption

$$MDEA + CO_{2(l)} + H_2O \rightleftharpoons MDEAH^+ + HCO_3^- \quad (14)$$

Mineralisation

$$Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3 \downarrow \quad (15)$$

Amine regeneration

$$MDEAH^+ \rightleftharpoons MDEA + H^+ \quad (16)$$

The bicarbonate generation mechanism is negligible in primary and secondary amine as carbamate formations take place more quickly than bicarbonate formations. In this research, researchers prefer to use amines involving bicarbonate formation during CO_2 absorption as this study aims to use amines mainly in cement chemistry. Bicarbonate formation amines lead to form calcium carbonates from $Ca(OH)_2$ and C-S-H and hence enhance the strength.

Table 2 Reactions and corresponding equilibrium constants at 298.15K

Reaction No.	Equilibrium constant $\log_{10} K$
11	3.508 [9]
13	−9.868 [9]
14	2.187 [5]
16	-10.291[5]

Even though the carbamate of AEEA could be hydrolysed and form free amine and bicarbonates under high pressure, it will not be subjected to bicarbonate formation under atmospheric pressure. As the purpose of this research is to use amine in cement chemistry to capture CO_2 under atmospheric conditions, AEEA will not fulfil the expectation of this research team. Even though the system containing AEEA forms a small amount of bicarbonate due to the dissociation of CO_2 in H_2O, it is less than the systems without any amine. Consequently, MAE and MDEA are given much consideration, and the equilibrium constants of these reactions were calculated with the help of previous work and tabulated in Table 2.

3. MATERIALS AND METHODS

3.1 Materials

The reagents 2-(2-aminoethylamino)ethanol (AEEA, ≥98%), 2-(methylamino)ethanol (MAE, ≥97%) *N*-methyldiethanolamine (MDEA, ≥98%), and $Ca(OH)_2$ (special grade reagent) were purchased from Kanto Chemical Co., Inc, Japan, without further purification. SiO_2 (AEROSIL200 with a purity of 99.9% or higher) was purchased from Nippon Aerosil Co., Ltd and Ordinary Portland Cement (OPC) (Class (H), confirmed to the Japan Industrial Standard JIS R 5201:2015) was purchased from Japan Cement Association. C-S-H was synthesised using $Ca(OH)_2$ and SiO_2 with a Ca/Si ratio of 1.0.

3.2 Experimental Procedure

The CO_2 mineralisation experiment was carried out as shown in Fig.1. Three amines (AEEA, MAE and MDEA) were selected, and the CO_2 capturing capacity of each amine was tested with different Ca-rich materials such as $Ca(OH)_2$, C-S-H and hydrated cement powder. C-S-H was synthesised, and hydrated cement powder was obtained by grinding hardened cement paste. Firstly, a Ca-rich solution was prepared by mixing selected amine, water and different Ca-rich materials. The dosage of Ca-rich material was defined as (10 mL/g) 1.0 g of Ca-rich material was added with 10 mL of amine aqueous (amine+water) solution. The different amine concentration was selected to study the effect of amine percentage on carbonation. The amine percentages of 0%, 5%, 10% and 20% of the total volume of aqueous amine solution were selected. The volume of the aqueous amine solution was 300 mL. The solid particles were well mixed with the aqueous amine solution by a stirrer. The resulting Ca-rich solution was subjected to carbonation in the environment where the relative humidity was at 60 ± 10% and the temperature at 20 ± 2˚C. CO_2 was applied with a concentration of 5 vol% and a flow rate of 2 L/min for a specific time. Carbonation time was selected after conducting the sensitive study by changing the carbonation time to observe the apparent result of carbonation.

After carbonation, the solid and liquid phases were separated using a suction filter. The liquid phase was subjected to pH analysis, and the powdered solid phase was subjected to several analyses after drying at 40˚C for 24 hours.

3.3 Characterisations

Synthesised C-S-H was characterised by X-Ray Diffraction (XRD), X-Ray Fluorescence (XRF), Thermogravimetric Analysis (TGA) and Scanning Electron Microscope (SEM). The hydrated cement powder was subjected to TGA to quantify the portlandite before carbonation. And the solid phase, separated by filtration after carbonation, was subjected to several analyses, such as XRD, TGA and SEM, to identify and quantify the solid phase composition. The liquid phase was subjected to pH analysis.

4. RESULTS AND DISCUSSION

4.1 Characterisation of Synthesised C-S-H and Hydrated Cement Powder

Synthesised C-S-H was characterised before use. XRD pattern of synthetic C-S-H is shown in Fig.2. Diffraction peaks at eight different 2θ positions (7.06°, 16.71°, 29.06°, 31.94°, 43.04°, 49.79°, 54.94° and 66.76°) were identified as the representative reflections of C-S-H. The high purity of C-S-H was confirmed as no other phases were found in the XRD pattern.

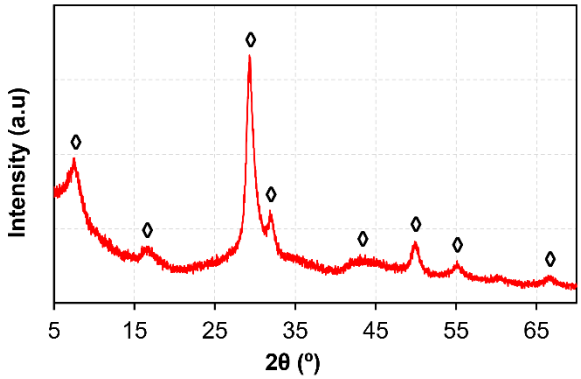


Fig.2 XRD pattern of synthetic C-S-H

The measured Ca/Si ratio by XRF and SEM elemental analysis was 0.9 and 1.1, respectively. This result shows less deviation (±0.1) from the target value (1.0). TGA analysis was carried out for synthesised C-S-H, and its purity was confirmed as there was only decomposition of C-S-H in the TGA curve. $Ca(OH)_2$ present in the hydrated powder before CO_2 mineralisation was quantified as 21% (by weight) by TGA.

4.2 Optimisation of CO_2 Mineralisation

A parametric study was carried out before selecting parameters such as water/powder ratio, amine concentration, and carbonation time. The water/powder ratio and carbonation time were chosen to observe and compare the CO_2-capturing ability of different amines in different Ca-rich materials. The water/powder ratio was selected as 10 mL/g, and the different carbonation period was chosen for different Ca-rich material as the concentration of Ca^{2+} varies, hence carbonation rate changes. The carbonation time for $Ca(OH)_2$ was two hours, and for C-S-H and hydrated cement powder, it was six hours. When the carbonation period of two hours was applied to C-S-H and hydrated cement powder, no significant change was observed after carbonation. While the carbonation period of six hours was used for $Ca(OH)_2$, no remaining $Ca(OH)_2$ was observed. The selected carbonation time and water/powder ratio were adequate for the noticeable changes in the carbonation in the presence of different amines. As this study intends to find the better solvent for CO_2 capture in cement-based material, the same experimental condition was applied for all three amines in specific Ca-rich material.

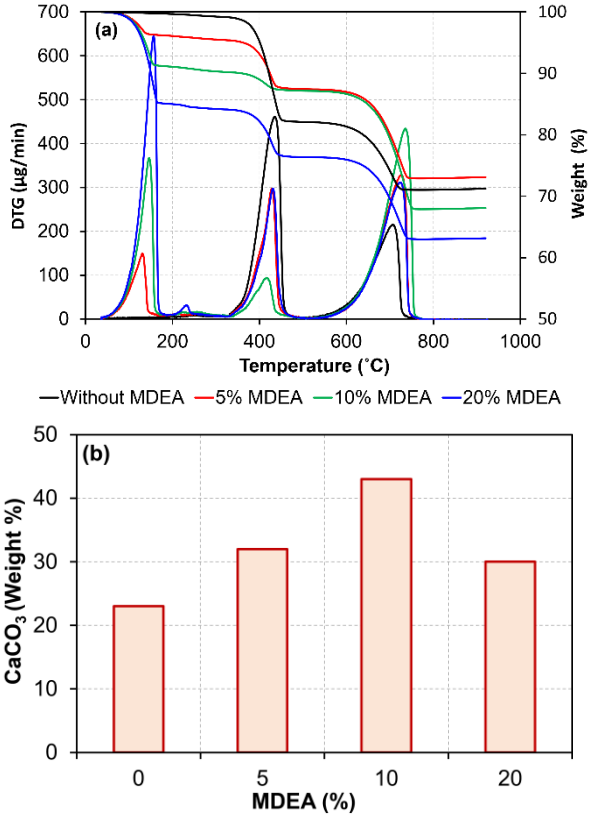


Fig.3 Effect of MDEA amine percentage on the CO_2 mineralisation in $Ca(OH)_2$ (a) TGA curves (b) Quantitative results from TGA

The influence of the percentage of amine was studied in the aqueous amine solutions with $Ca(OH)_2$. The amine percentages of 0%, 5%, 10% and 20% were selected. The comparison of the effect of amine percentage on CO_2 mineralisation is shown in Fig.3. The extent of CO_2 mineralisation during carbonation was determined by measuring the quantity of $CaCO_3$ precipitated. The weight percentage of $CaCO_3$ was measured by employing TGA analysis. The rate of carbonation increases as the proportion of amine rises, up to a maximum of 10%, as shown in Fig.3(b). This can be explained by the fact that a higher concentration of amine molecules leads to the greater formation of bicarbonate. However, when the amine proportion exceeds 10%, the rate of carbonation decreases due to a reduction in the availability of $Ca(OH)_2$ for the reaction. This reduction is caused by a more significant loss of amine on the surface of $Ca(OH)_2$, as observed through TGA analysis, as shown in Fig.3(a). Consequently, a 10% amine concentration was used for the remainder of

the study to investigate the optimal solvent for CO_2 mineralisation in cement-based materials.

4.3 Mapping of Different Amines for CO_2 Mineralisation

The influence of three selected amines, AEEA, MAE and MDEA, on CO_2 mineralisation, pH and formation of polymorphs of $CaCO_3$ was studied. Each amine was tested under identical operating conditions to ensure differences in results were due to its properties.

(1) Effect of amine type on CO_2 mineralisation

Effect of different types of amines, such as primary and secondary amine (AEEA), secondary hindered amine (MAE), and tertiary amine (MDEA), on CO_2 mineralisation was studied in the presence of different Ca-rich materials such as $Ca(OH)_2$, C-S-H and hydrated cement powder.

Figure 4 depicts a comparative analysis of the weight percentage of $CaCO_3$ obtained from thermogravimetric analysis (TGA) results. The experimental investigation encompassed diverse amines that were employed to facilitate carbonation in cement-based materials. The graphical illustration is indicative of the substantial influence of different amines on the resultant amount of $CaCO_3$ precipitate in various Ca-rich materials. Notably, it is discernible that among all the amines tested, MAE elicits the highest degree of $CaCO_3$ precipitate, as reflected in the figures of 53%, 36%, and 32% for $Ca(OH)_2$, C-S-H, and hydrated cement powder, respectively. These results highlight the significance of the selection of suitable amines in promoting the carbonation process in cement-based materials and further underscore the potential of MAE as a promising agent for enhancing the carbonation performance of such materials. This superiority can be attributed to several factors, chief among which is its relatively higher reaction rate compared to other amines. Furthermore, stoichiometric considerations suggest that the conversion of carbamate to bicarbonate is favoured in the case of MAE, thus leading to an improved rate of CO_2 absorption. It is worth noting that MAE belongs to the category of sterically hindered amines, which are characterised by having a bulky substituent close to the amino group. This structural feature can decrease the stability of carbamate and weaken the N-H bond, resulting in greater hydrolysis and bicarbonate formation and hence higher $CaCO_3$ formation. Therefore, the unique chemical properties of MAE make it a promising candidate for enhancing the carbonation performance of cement-based materials and merit further investigation in this field.

Moreover, MDEA gives more $CaCO_3$ than the control samples (without any amine) in all three Ca-rich materials, albeit lower than the yield obtained with MAE, as shown in Fig.4. The underlying reason for this phenomenon can be attributed to the fact that MDEA serves as a sink for protons produced by the slow CO_2 hydrolysis process. However, this slow hydrolysis leads to the formation of more bicarbonates than the control samples. The results indicate that MDEA yielded 1.9, 4.2, and 2.2 times calcite compared to control samples in $Ca(OH)_2$, C-S-H, and hydrated cement powder, respectively.

It is evident from the results indicated in Fig.4 that there is an amine that gives less amount of $CaCO_3$ precipitate than the system without any amine. Especially, AEEA gives a minimal amount of $CaCO_3$ precipitate, indicating no $CaCO_3$ production in the presence of this amine. This is proven by the reaction mechanism mentioned in section 3.1. As AEEA has a primary and a secondary amine, it mainly forms carbamate instead of bicarbonate ions during CO_2 mineralisation.

From these results, as AEEA gives less $CaCO_3$ precipitation, it is considered an unsuitable solvent for CO_2 capture in cement-based materials. The amines that form $CaCO_3$ during carbonation are preferred as precipitation of $CaCO_3$ is expected to balance the chemical and mechanical properties after adding the amine. Therefore, AEEA was not considered to study with C-S-H and hydrated cement powder.

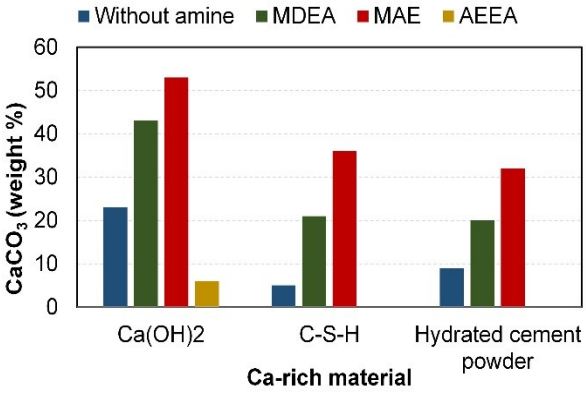


Fig.4 Effect of amine type on the CO_2 mineralisation in Ca-rich materials

Although $CaCO_3$ still forms in the system without any amine as a result of bicarbonate formation from CO_2 dissolution, the quantity produced was lower compared to the systems that contained MAE and MDEA.

(2) Effect of amine type on the formation of polymorphs of $CaCO_3$

$CaCO_3$ crystal nucleate and crystal growth are affected by the presence of amino groups as they are organic additives, and their ability to complex with carbonate ions will vary with different amine structures. They have a significant effect on the formation of polymorphs of $CaCO_3$. Therefore, studying amine's impact on the formation of polymorphs is inevitable in this research.

Calcite, aragonite and vaterite are the polymorphs of $CaCO_3$. Many factors, such as pH, ion concentration of Ca^{2+} and CO_3^{2-}, temperature, and organic addition [1], affect the formation of polymorphs. Fig.5 summarises the effect of amines on the formation of polymorphs of $CaCO_3$ and the pH of the solution after carbonation in htdrated cement powder. Fig.5(a) shows the XRD pattern of hydrated cement powder after carbonation, and it can be seen that adding amine forms aragonite (peak marked within the red colour box). This is

confirmed by SEM images shown in Fig.5(b). Arogonite (needles shape) together with calcite (cubic, Rhombic, and polygonal plate-like crystal) is observed when the amine is introduced. In contrast, pure calcite is formed if there is an absence of amine, which coincides with the previous research [1]. As the molar weight of aragonite (2.94 g/cm^3) is higher than that of calcite (2.71 g/cm^3), adding amine is favourable in cement-based materials in terms of forming polymorphs of $CaCO_3$.

In addition, the pH of a solution can affect carbonation by altering the concentration of carbonic acid in the solution. The pH of the initial solution changes due to the addition of amine. While this study did not directly investigate the effect of pH on carbonation in cement-based materials, the pH values observed after carbonation are above 9 (shown in Fig.5(b)), which is higher than 8.6 as cement paste no longer provides a passive environment for embedded steel at approximate pH of 8.6. Upon selecting an appropriate amine, the corresponding amine will undergo testing with cement paste, mortar, and concrete to conduct further investigations for potential real-world applications.

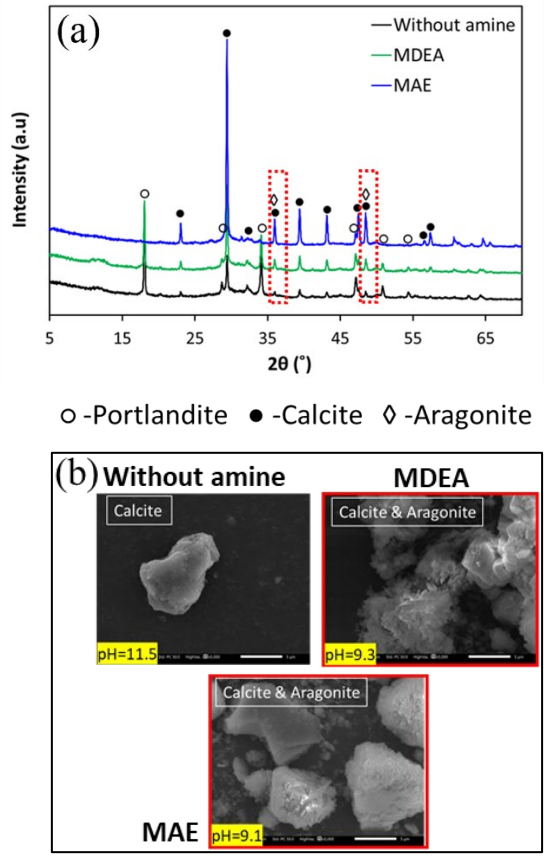


Fig.5 Effect of amine type on the formation of polymorphs of $CaCO_3$ in hydrated cement powder (a) XRD result (b) SEM images and pH

5. CONCLUSIONS

In conclusion, this study investigated the effect of three different types of amines on the CO_2 mineralisation process and the formation of polymorphs of $CaCO_3$. MAE captured the highest amount of CO_2 and gave the highest amount of precipitation of $CaCO_3$ in all three Ca-rich solutions, followed by MDEA and a system with no amine. AEEA failed to provide the $CaCO_3$ precipitate as it forms carbamate ions instead of bicarbonate ions during carbonation. Moreover, amine influenced the formation of polymorphs of $CaCO_3$. Adding amine led to the form of aragonite (which has a larger molar weight than the other two types of polymorphs) type of polymorphs together with calcite, while the absence of amine led to the form of pure calcite. However, more in-depth studies could be conducted to investigate the effect of other variables on the process, such as the pH effect on carbonation and to study the applicability of this procedure for cement paste, mortar and concrete. Such studies could help in further optimising the process for industrial applications.

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