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Biodegradable carboxymethyl inulin as a scale inhibitor for calcite crystal growth: Molecular level understanding

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HIGHLIGHTS

- Investigate interaction of CMI and calcite by molecular dynamics simulation
- CMI has strong interactions with calcite and possesses superior inhibitory.
- Aqueous environment weakens interactions between CMI and calcite.
- Molecular dynamics simulation is a very useful guide on calcite inhibitor design.

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ABSTRACT

Carboxymethyl inulin (CMI) is one of the most promising biomass materials for scale inhibition. Its potential applications as a scale inhibitor have attracted much research attention. Understanding the interactions between CMI and calcite surfaces is very important for the design of scale inhibitors. In this study, molecular dynamics simulations were carried out to investigate effects of temperature, CMI chain length, and calcite cleavage on the interactions between CMI and calcite. The results indicate that for the same mass of CMI (with different degrees of polymerization, n = 1, 3, 5), CMI exhibits different abilities in inhibiting the growth of calcite crystal in the order of CMI (n = 5) > CMI (n = 3) > CMI (n = 1) for calcite (012), (104), ($1\bar{1}0$), and (110) surfaces. For the calcite (012) surface, the inhibition ability is similar for CMI (n = 3) and CMI (n = 5). For the aqueous environment, comparison of the results of water effects with the results for the CMI–calcite surfaces without water showed a similar trend: the interaction between the CMI and the calcite (012) surface was greater than that of the CMI with the other calcite surfaces (104), (110), and ($1\bar{1}0$). However, the interactions between the CMI and the other calcite surfaces (104), (110), and ($1\bar{1}0$) were apparently weakened by the water environment. The results also show that temperature influences the interactions between CMI and calcite surfaces. This study provides important information for CMI potential applications as calcite inhibitor.

1. Introduction

Water attracts considerable attention as one of the most important substance in our daily life. Much scientific work is related to water pollution, waste water treatment, and scale during the processes of water usage. The growth of scales is commonly prevented or slowed by the use of scale inhibitors [1–2]. So far, scale inhibitors extensively used in water systems are mainly acrylic acid polymers, maleic acid polymers, and phosphonates. These agents are widely used because of their excellent properties of scale inhibition, such as good solubility threshold effect, low dosage effect, and high temperature endurance [3–4]. Investigations have been undertaken to study the influence of scaling inhibitors on both the precipitation and crystal behavior modification of calcium carbonate polymorphs [3–7].

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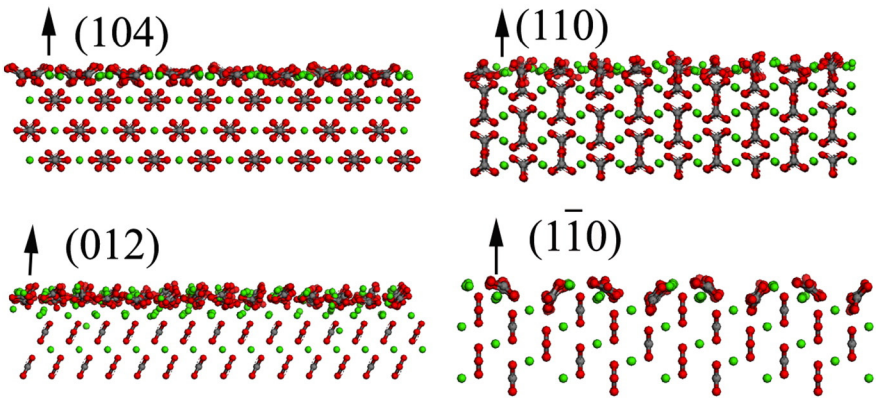

Fig. 1. Optimized geometry of the different calcite surfaces after annealing (ball and stick model, color codes: calcium, green; oxygen, red; carbon, gray). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Polysaccharides are polymeric carbohydrate structures that are made of monosaccharide units bound together by glycosidic linkages. They have attracted much research interest because of their non-toxic, renewable, and biodegradable properties, and these specific properties meet the requirements of biomaterials or environmentally friendly materials [8–9]. Carboxymethyl inulin (CMI), as one of the polysaccharides that can be isolated from the roots of *Inula helenium*, is inherently biodegradable [10]. CMI is free of nitrogen and phosphor and its very low aquatic toxicity has been identified [12]. CMI has been used in oil exploration, for drug delivery systems, and also as a crystal growth inhibitor [10–13]. It has been shown that CMI is a very effective inhibitor of calcite crystal growth. Kirboga et al. [12–13] found that CMI could induce the

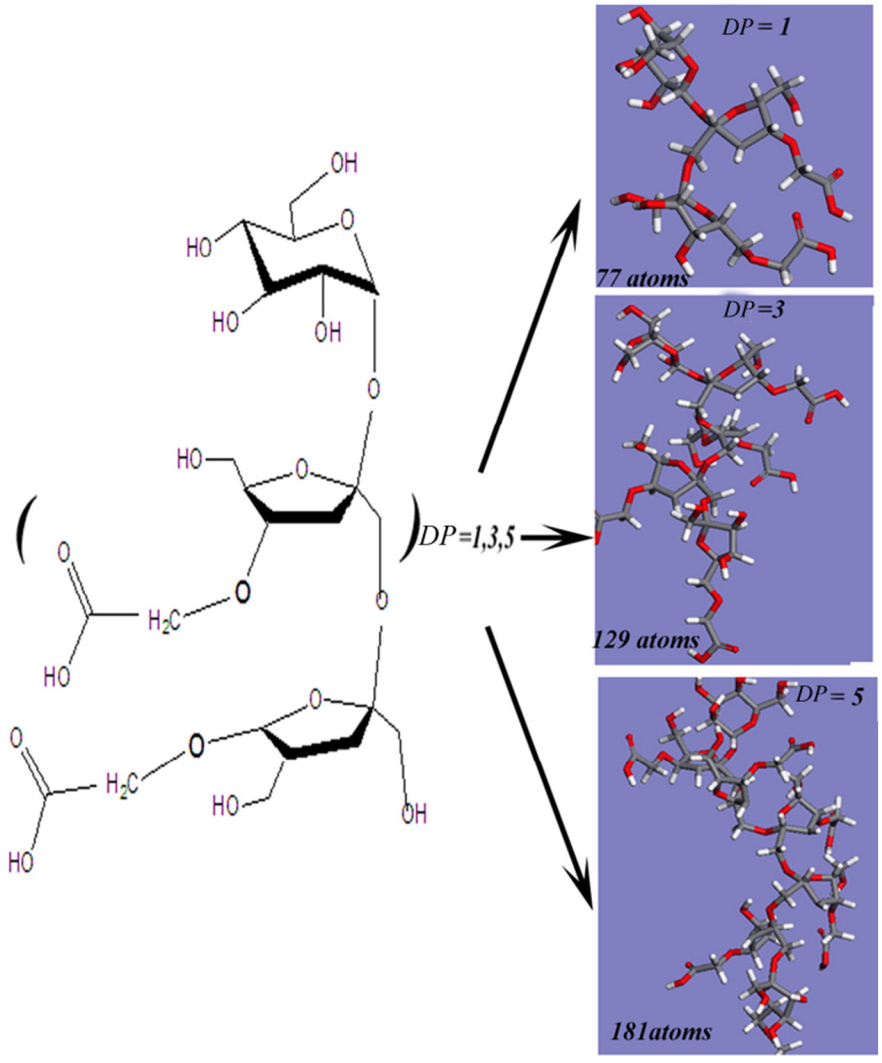

Fig. 2. Schematic and simulation models of carboxymethyl inulin (CMI) with different numbers of repeat units (color codes: hydrogen: white; oxygen, red and carbon, gray). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)