

Dynamic CO₂ sorption on MgO-based sorbent in the presence of CO and H₂O at elevated pressures

MgO-based sorbents have received a great attention as a sorbent for pre-combustion CO₂ capture. Still, few studies have been conducted on how the sorption mechanism varies in the presence of gases other than CO₂. Here, we report on the dynamic CO₂ sorption behavior of MgO-based sorbents under simulated practical conditions, including H₂O and CO.

The CO₂ sorption behavior of the salt-promoted MgCeO_x prepared by a sol-gel combustion-assisted method was examined in the fixed bed reactor by monitoring the breakthrough of effluent gases (CO₂, CO, Ar) with an on-line mass spectrometer (**Hidden HPR 20**). The breakthrough experiments under various practical relevant conditions indicated that the feed gas composition was a dominant factor in determining the dynamic CO₂ sorption behavior (Figure 1), whereas the breakthrough profiles was not significantly influenced by the sorption temperature conditions. When H₂O was included up to 60% in the feed gas (wet condition), the breakthrough time increased significantly from 159 sec to 213 sec compared to the dry condition (Figure 1(a)). Even under the wet condition, the presence of CO in the feed condition resulted in the immediate breakthrough of a trace amount of CO₂ and decreased the CO₂ sorption capacity of the sorbents (Figure 1(a)). Based on the understanding of dynamic CO₂ sorption behavior from the breakthrough experiment, the underlying sorption mechanisms influenced by H₂O and CO molecules were studied via *in situ* DRIFTS analyses under various CO₂ mixtures.

In *in situ* DRIFTS (Diffuse Reflectance Infrared Fourier-Transform Spectroscopy) analyses where the change of OH groups generated by the presence of H₂O was observed, the peak intensities of multi-coordinated and mono-coordinated OH groups in the wet conditions increased by 2.32 and 1.72 times, respectively, compared with those in the dry conditions. These results indicated that the surface OH groups were developed by the dissociation of H₂O at the oxygen vacancies on the MgCeO_x surface, which were subsequently occupied by the OH groups (Figure 2(a)). In particular, compared with other surface species, the peak intensities of the adsorbed OH groups and monodentate carbonate in wet conditions increased at remarkably high rates. The results suggested that H₂O may function as a crucial component in the initial rapid sorption of CO₂, allowing CO₂ to be bound in the form of monodentate carbonate.

To understand the immediate breakthrough of CO₂ in the presence of CO, the CO₂ pulse titration experiments were conducted by exposing the MgCeO_x sorbent to the dilute CO flow, purging with the inert gas, and analyzing generated gases with the mass spectrometer during the consecutive CO₂ pulses. The result revealed that the interrupted CO₂ sorption in the co-existence of CO and H₂O was caused by competitive sorption (Figure 1(b) and Figure 2(b)). First, the WGS (Water-Gas Shift) reaction was catalyzed by MgCeO_x to generate CO₂. Then, CO and the WGS-induced CO₂ competitively occupied the sorption sites where CO₂ in the feed gas could have been sorbed, thereby hindering initial rapid CO₂ sorption.

This study showed the approach to understand the dynamic sorption behavior by coupling the result from the breakthrough experiment and the *in situ* DRIFTS and the obtained result can give a guide to overcome the obstacles for the ultimate application of MgO-based sorbents.



Hidden HPR-20 Mass Spectrometer

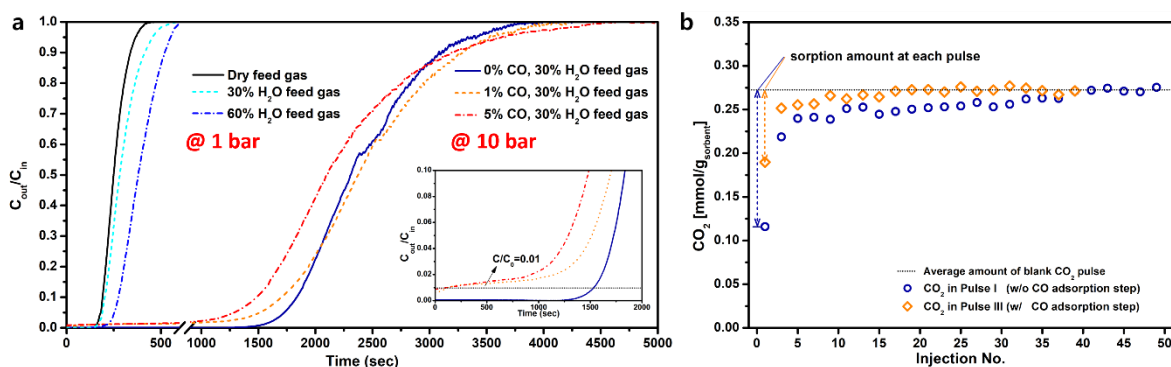


Figure 1. (a) CO₂ breakthrough experiments at different pressures under feed mixtures flow including H₂O and/or CO and (b) CO₂ pulse titration experiments with (Pulse III) and without (Pulse I) CO adsorption step for salt-promoted MgCeO_x.

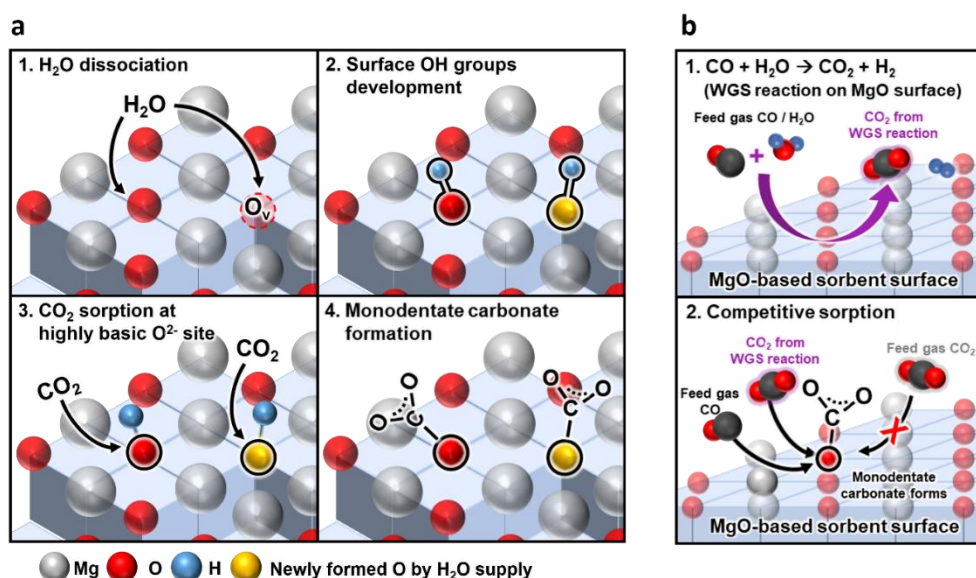


Figure 2. Schematics of CO₂ sorption mechanism (a) in wet CO₂ condition and (b) in wet CO₂/CO condition on the surface of MgO-based sorbent.

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Hidden Product:

[HPR-20](#)