Film thickness and its relationship with CO_2 adhesion on mineral surfaces

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Film Thickness on Different Silica Surfaces

We show that water film thickness decreases as contact angle increases. The predicted thickness is smaller than experimental results because we used flat silica surfaces and film thickness decreases as surface roughness decreases [1].

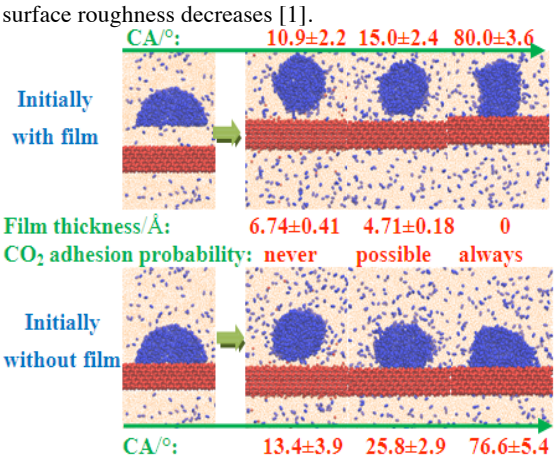

Figure 1: Snapshots of simulation systems (20MPa and 313K) as well as an illustrtion of film break mechanism of CO_2 adhesion on mineral surfaces. Three different silica surfaces were used (from left)[3]: Q^3-50%, Q^3 and Q^3/Q^4.

A Mechanism of CO_2 Adhesion on Mineral Surfaces

CO_2 adhesion may be caused by water film break leading to contact angle increase: (1) at low CA conditions, no adhesion occurs as CO_2 droplet detachs even it was initially placed on surface without water film; (2) at high CA conditions, adhesion always occurs as film thickness tends to zero; (3) at mediate CA conditions, adhesion occurs with a possilibity which is controlled by film thickness. Adhesion incidence decreases as surface roughness increases [2] because of film thickness increasing [1]. Reacted biotite surfaces are more hydrophilic and exhibit a lower CO_2 adhesion [4] because of larger film thickness.

[1] Kim (2012) *Water Resour. Res.* **48**, W09558. [2] Wang (2013) *Environ. Sci. Technol.* **47**, 11858. [3] Chen (2015) *Environ. Sci. Technol.* **49**, 14680. [4] Zhang (2016) *Environ. Sci. Technol. Lett.* 10.1021/acs.estlett.5b00359