Wettability, Anti-Viral Treatments, and Potholes

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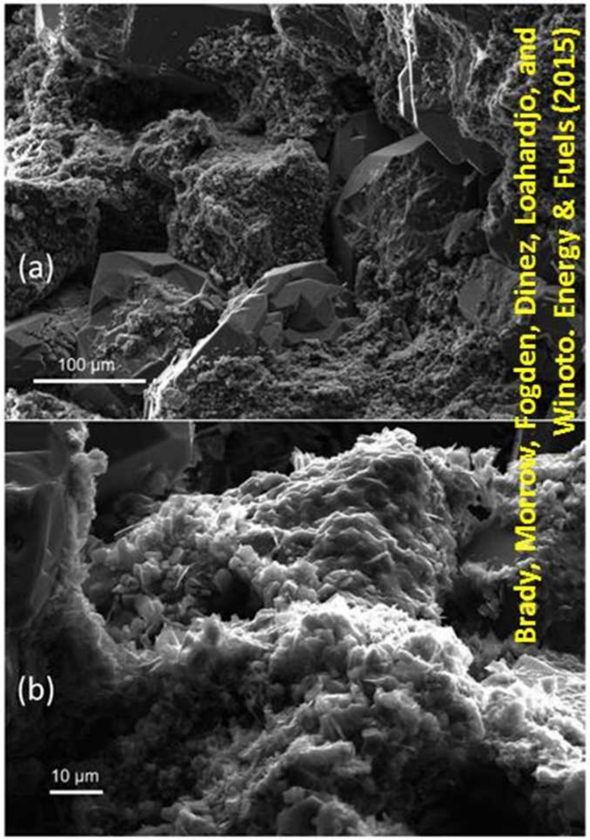
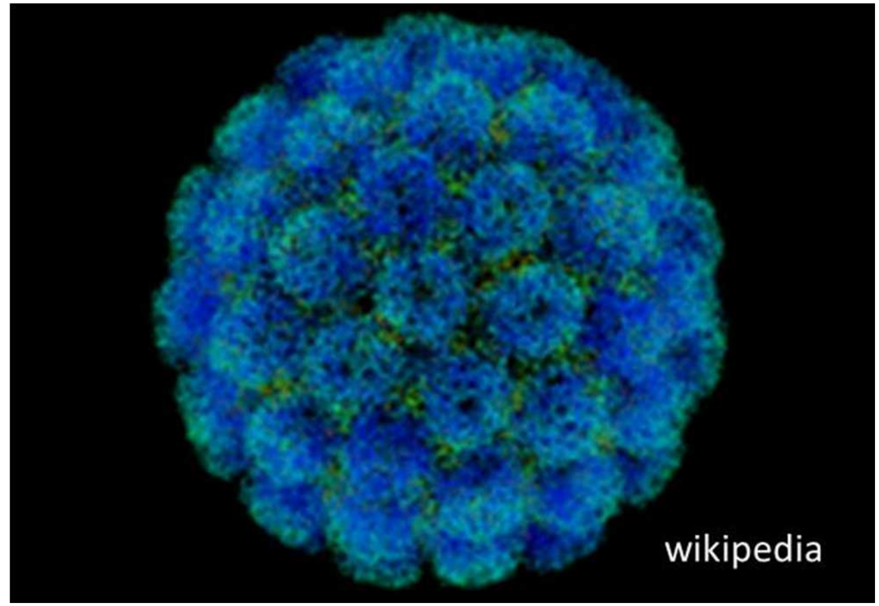
SAND2017-6341PE





Oil|Virus|Asphalt -NH^+ --- ^-O- Rock|Cell|Aggregate

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… *in the April 30, 2016 issue of The Economist*

Viral infections

General knowledge

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Progress towards a broad antiviral treatment

Apr 30th 2016 | From the print edition

… All viruses depend upon similar electrical charges at their surfaces to connect to the cells that they are trying to infect. If the charges on viruses and cells could somehow be meddled with, it should make things harder for the virus to infect the host…

IN THE medical armoury vaccines are a wonderful piece of ammunition. But they are like bullets that can hit one target only. Different vaccines are needed to prevent specific viral infections. If a person is already ill, vaccines won't help. Various antiviral drugs might, shortening the time people are ill or preventing serious complications. The trouble is viruses are a moving target because they can evolve rapidly. Researchers have tinkered with some antiviral treatments that might work against a wide spectrum of diseases, but all have had shortcomings. Now one group thinks they have found a method that might protect cells in the body from a viral invasion.

The new research, led by James Hedrick of the IBM Almaden Research Center in California, Naoki Yamamoto of the National University of Singapore and Yi Yan Yang of the Institute of Bioengineering and Nanotechnology, also in Singapore, stems from an old tactic that has been problematic in the past. All viruses depend upon similar electrical charges at their surfaces to connect to the cells that they are trying to infect. If the charges on viruses and cells could somehow be meddled with, it should make things harder for the virus to infect the host.

Lots of experiments have demonstrated that the theory is sound. Unfortunately, many of the materials used to interfere with the electrical charges have also been toxic to the cells they are supposed to protect. Dr Hedrick and his colleagues speculated that it might be possible to work around this problem with polyethylenimine. Previous work has shown

In this section

A printed smile

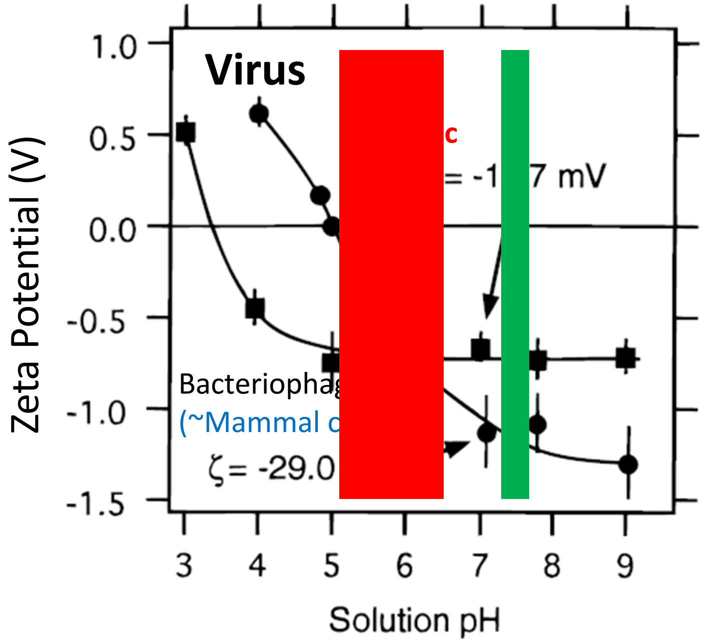
Getting the pulse racing

General knowledge

Buddy, can you spare a

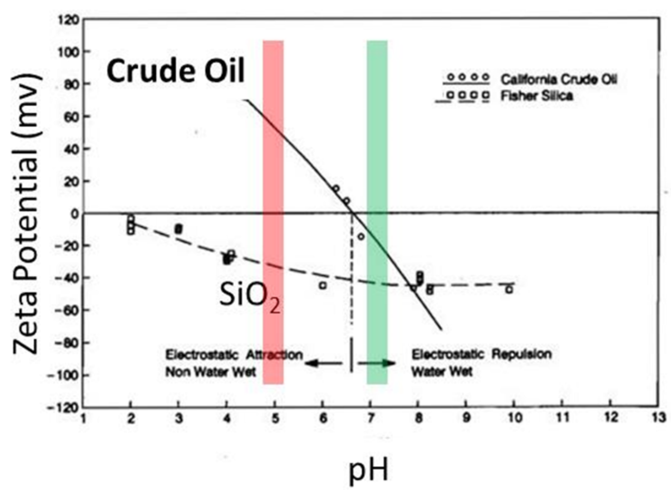
Endosomal pH 5-6.5 Physiological fluid pH 7.4

Virus on Cell



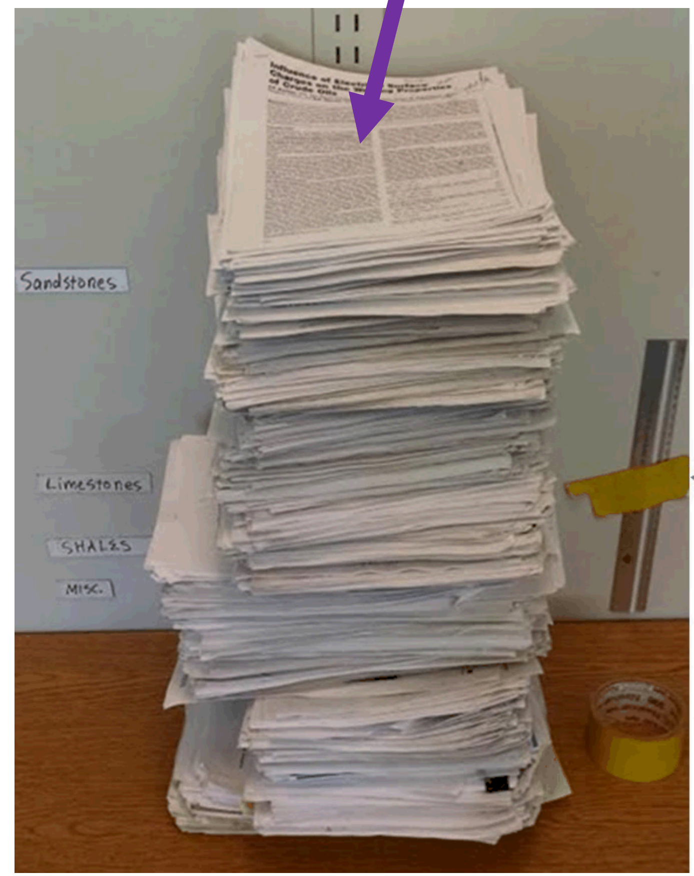
From Redman et al., 1997 ES&T

Oil on Rock



from Dubey and Doe (1993) *Base number and wetting properties of crude oil.* SPE Reservoir Engineering, 8 (195-200).

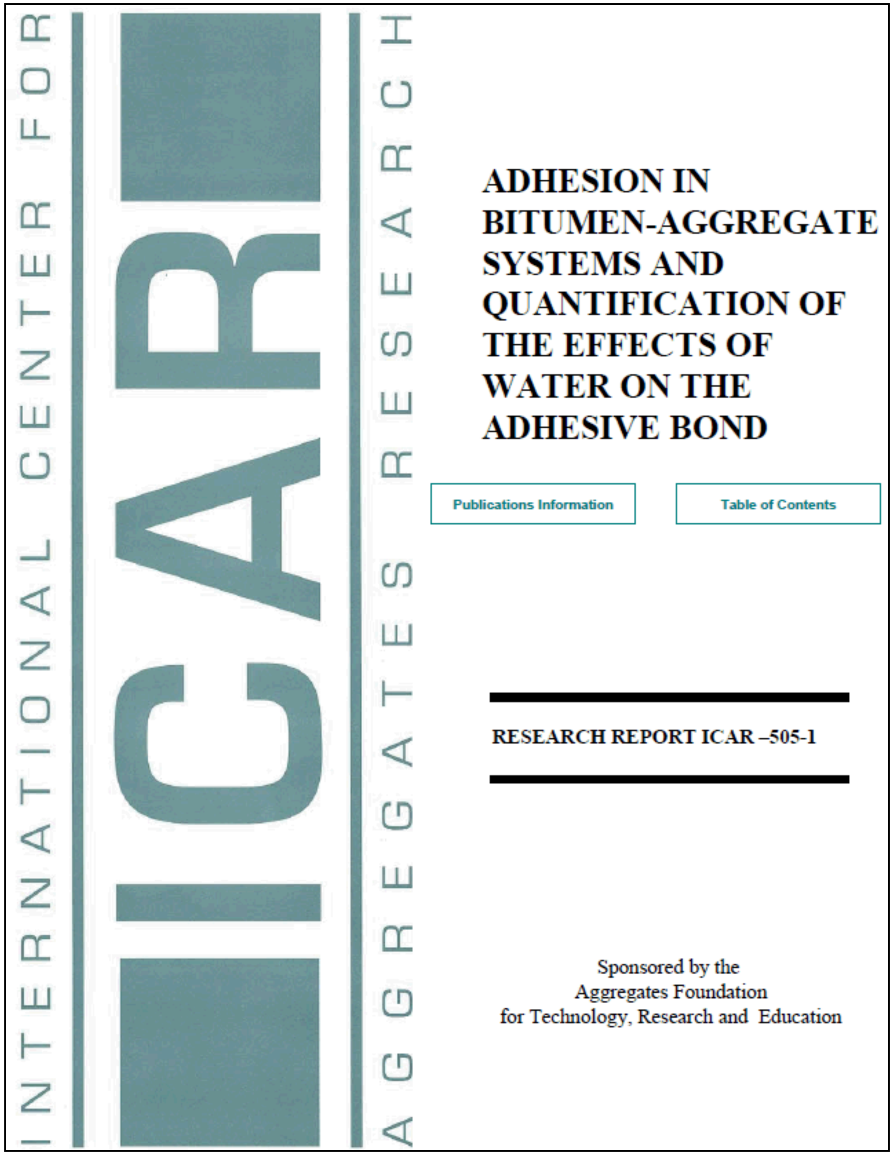
Dubey and Doe, 1993



12" ruler for scale

My stack of chemical waterflooding references

Pothole Formation


INTERNATIONAL CENTER FOR AGGREGATES RESEARCH

ICAR

ADHESION IN BITUMEN-AGGREGATE SYSTEMS AND QUANTIFICATION OF THE EFFECTS OF WATER ON THE ADHESIVE BOND

Publications Information

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RESEARCH REPORT ICAR –505-1

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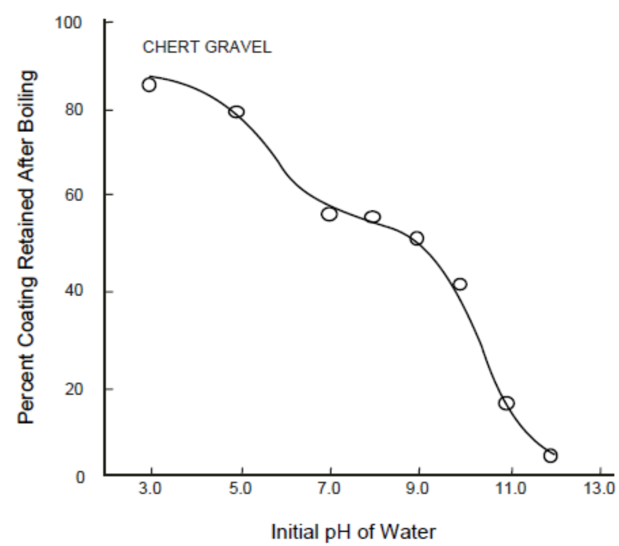
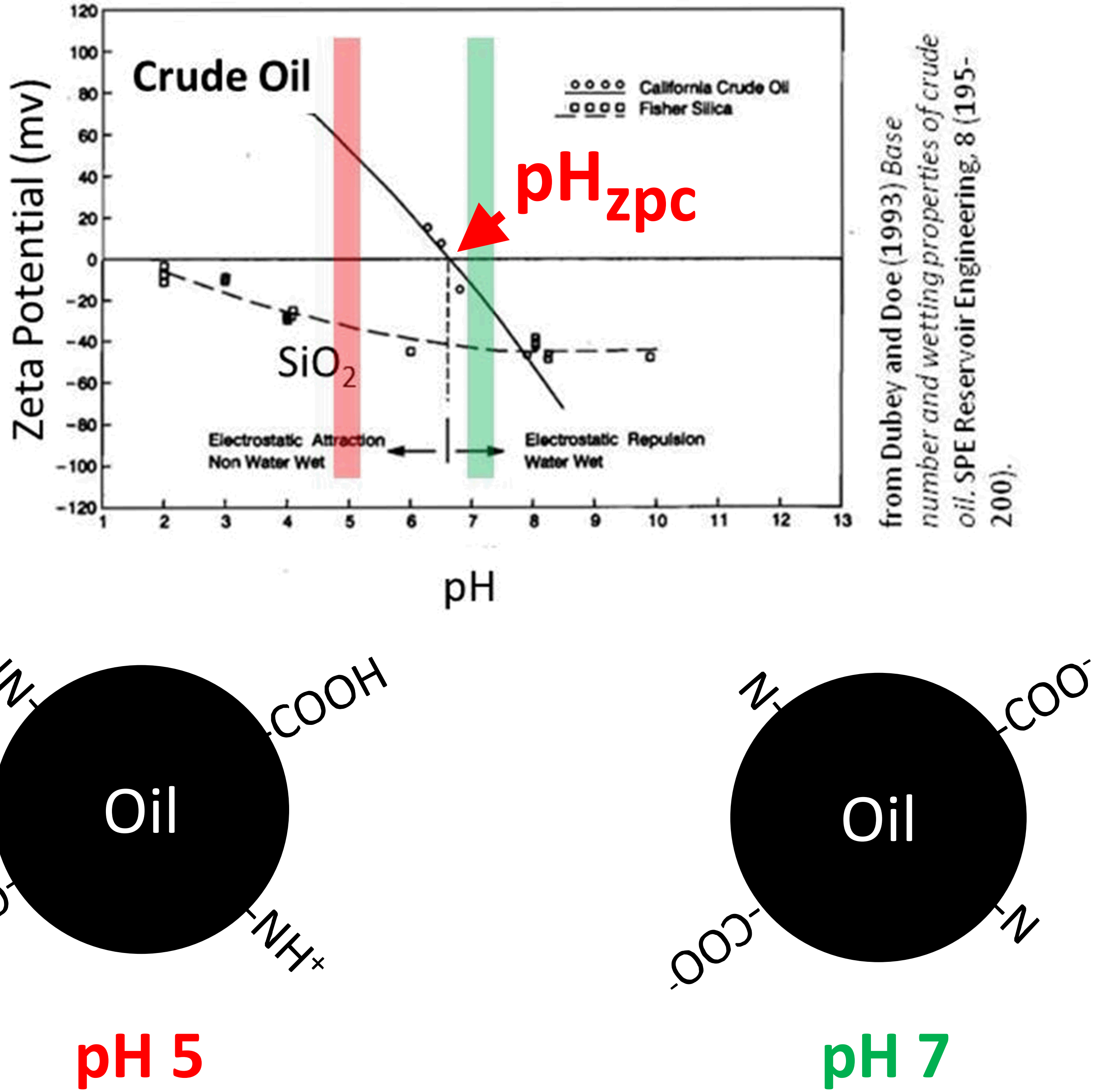
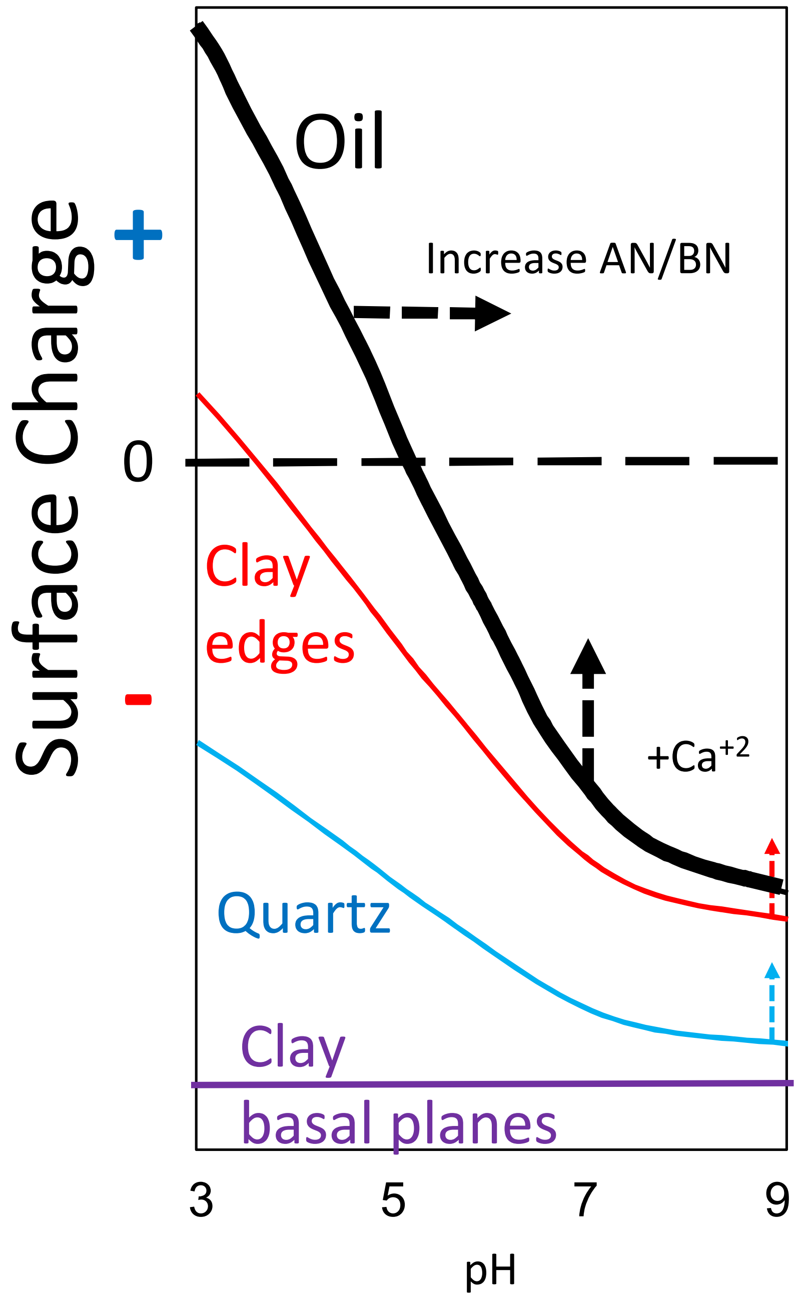
The addition of adhesion promoters to bitumen is common practice and numerous research papers and reviews have been published on different compounds used and the effects of anti-strip agents on performance of asphalt mixes. Basic, amine anti-strip agents are generally used to improve adhesion of bitumen with siliceous aggregates. Logaraj (2002) states that the two main characteristics of anti-strip additives are (a) they have a polar amine end group which will chemically bond with the siliceous aggregate surface, and (b) they have a hydrocarbon chain with similar properties to that of the bitumen so that they will interact and become part of the bitumen. A primary amine (RNH_2) and tertiary amine (NR_3) are schematically illustrated in Figure 15.





Crude Oil
California Crude Oil
Fisher Silica
pH
zpc
SiO2
Zeta Potential (mv)
pH
Electrostatic Attraction
Non Water Wet
Electrostatic Repulsion
Water Wet
from Dubey and Doe (1993) Base number and wetting properties of crude oil. SPE Reservoir Engineering, 8 (195-200).
+HN-
-COOH
HOOC-
-NH+
Oil
N-
-COO-
-COO-
-N
Oil
pH 5
pH 7



Oil

$-NH^{+} \leftrightarrow -N + H^{+}$

$-COOH \leftrightarrow -COO^{-} + H^{+}$

$-COOH + Ca^{+2} \leftrightarrow -COOCa^{+} + H^{+}$

Clay Edges

$>Al\text{-}O\text{-}H_2^{+} \leftrightarrow >Al\text{-}O\text{-}H + H^{+}$

$>Al\text{-}O\text{-}H \leftrightarrow >Al\text{-}O^{-} + H^{+}$

Quartz

$>Si\text{-}O\text{-}H \leftrightarrow >Si\text{-}O^{-} + H^{+}$

Clay Basal Planes

$Na + H^{+} \leftrightarrow >H + Na^{+}$

$>Na + -NH^{+} \leftrightarrow >-NH + Na^{+}$

$>Na + -COOCa^{+} \leftrightarrow >-COOCa + Na^{+}$

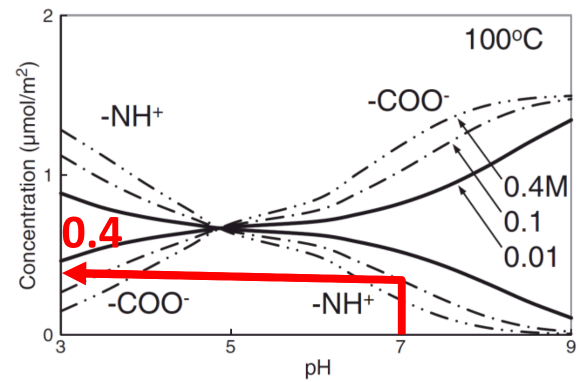
$2>Na + Ca^{+2} \leftrightarrow >Ca + 2Na^{+}$

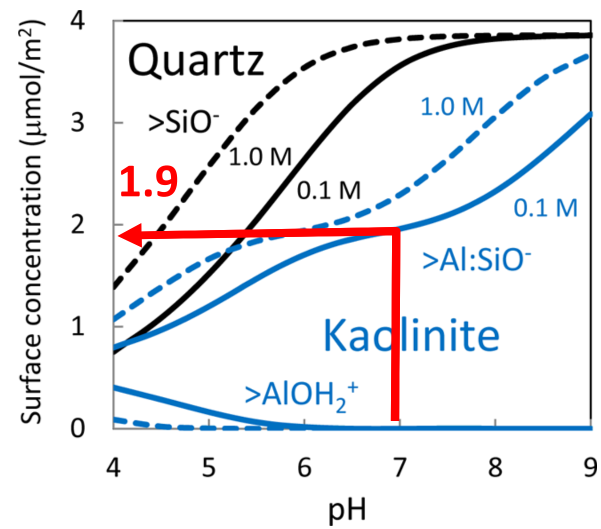
How to Model Oil-Rock Adhesion?

- Disjoining pressure
- Zeta potentials
- **Bond product sum**

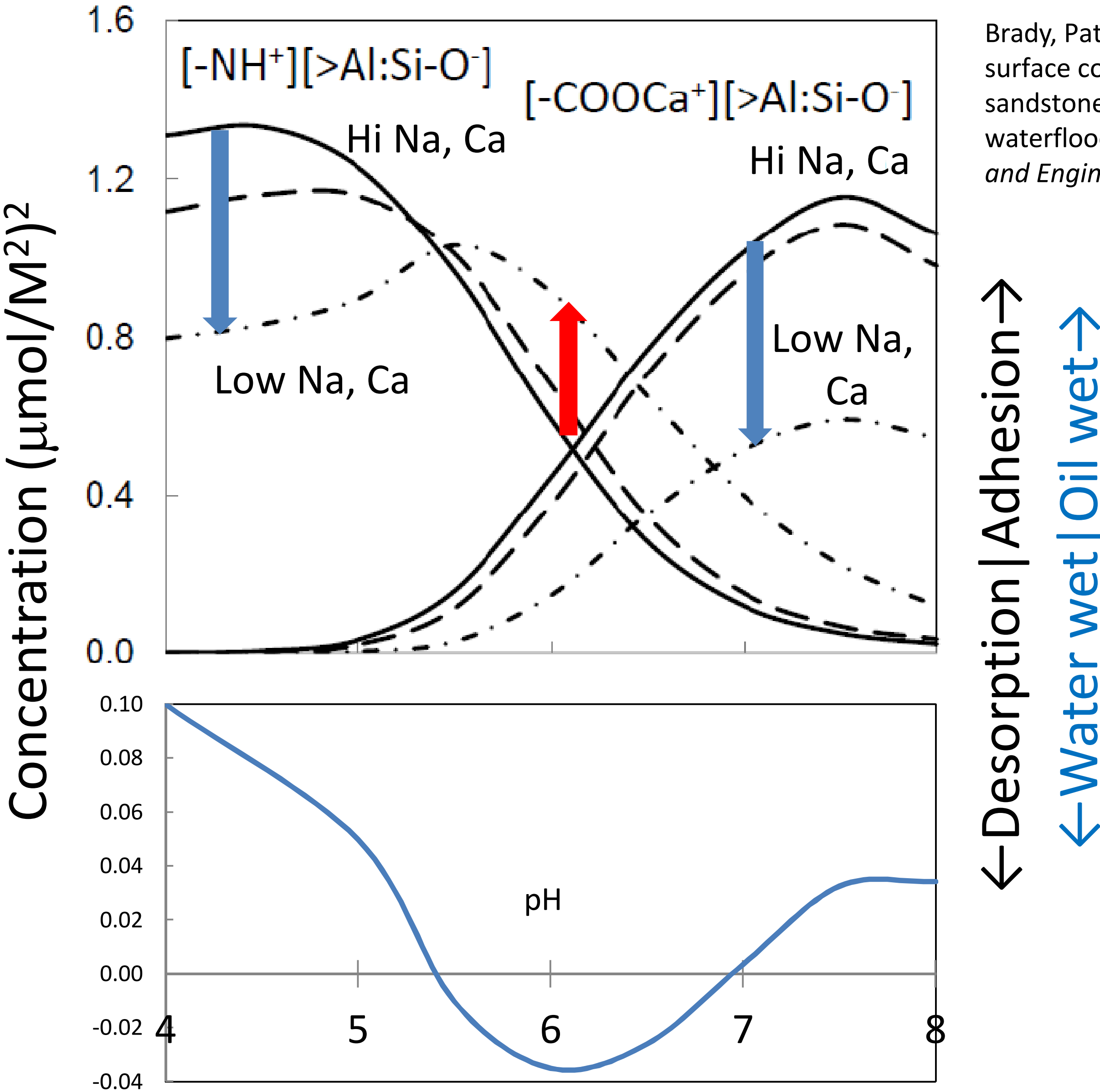
Example: Oil-NH^+ to Kaolinite >AlO^-, pH 7, 0.1M NaCl, 100°C.

Bond product = [-NH^+][>AlO^-] = 0.4*1.9 = 0.76 $(\mu mol/M^2)^2$

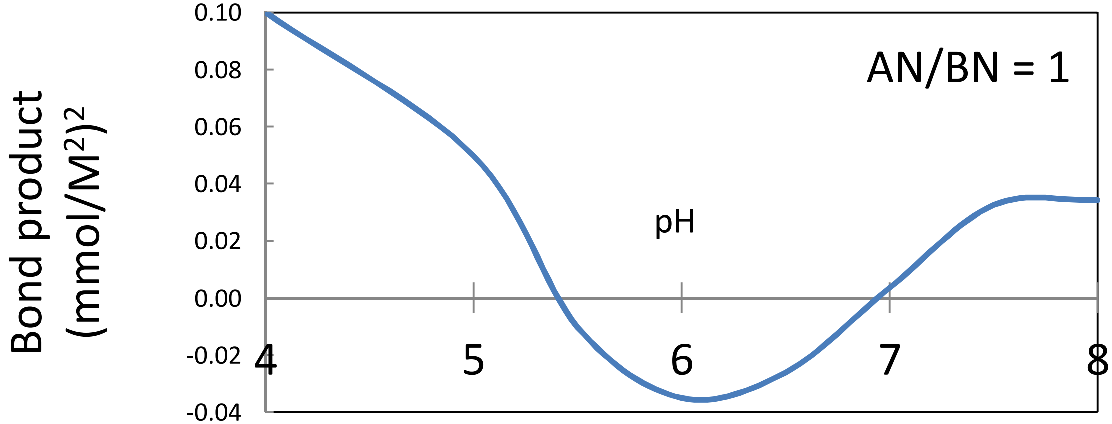


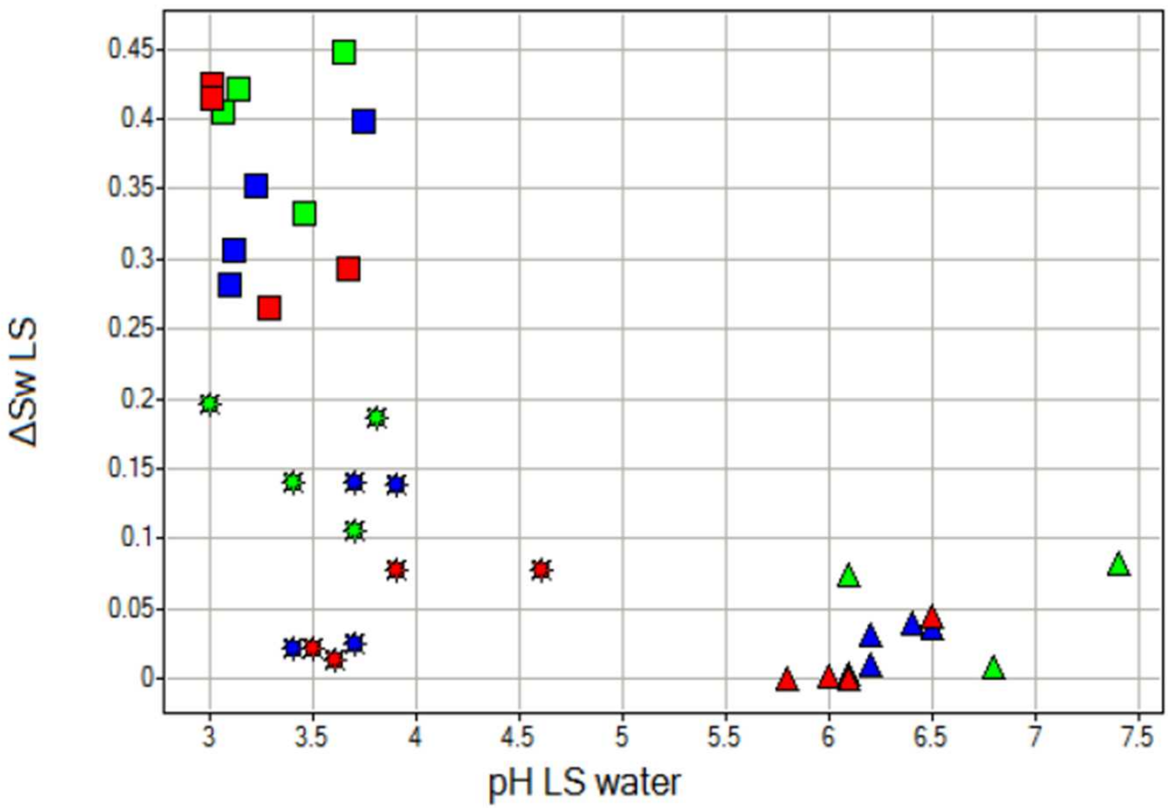


Kaolinite-Oil Adhesion



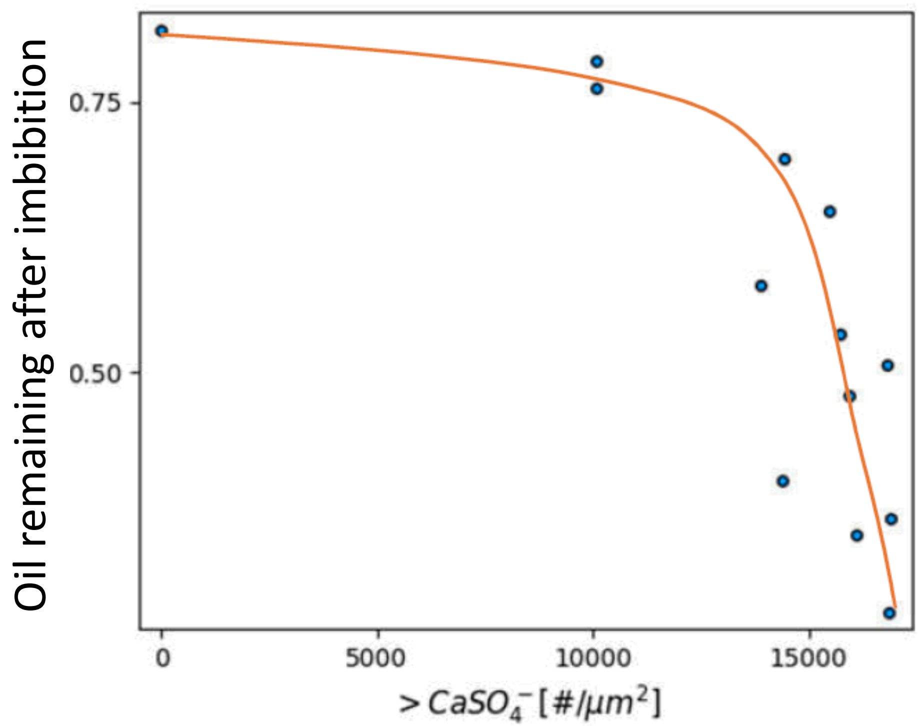
Brady, Patrick V., and James L. Krumhansl. "A surface complexation model of oil–brine–sandstone interfaces at 100° C: Low salinity waterflooding." *Journal of Petroleum Science and Engineering* 81 (2012): 171-176.

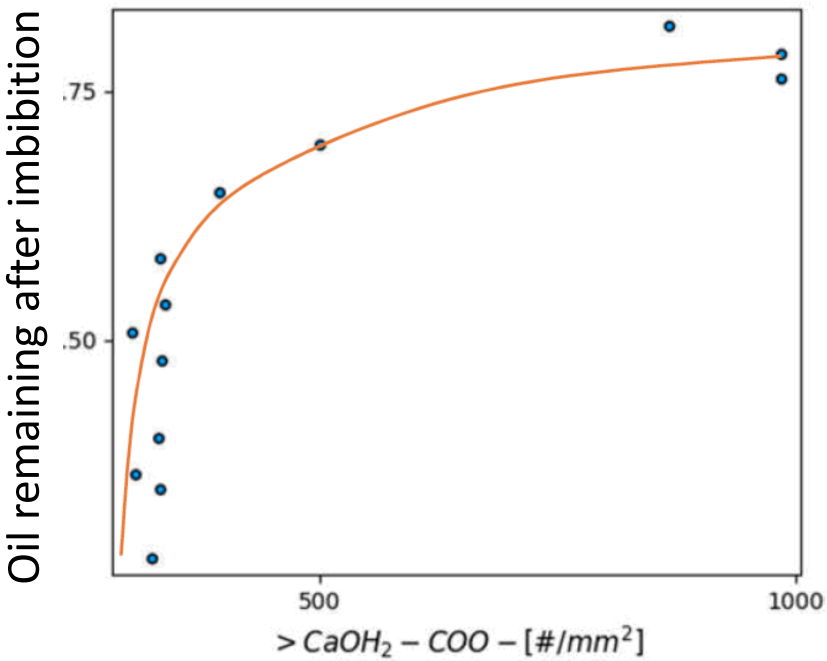




From: Van Winden, J. F., B. M. J. M. Suijkerbuijk, V. Joekar-Niasar, N. J. Brussee, H. A. van der Linde, A. H. M. Marcelis, A. H. Coorn, S. G. J. Pieterse, K. S. Ganga, and I. S. M. Al-Qarshubi. "The Critical Parameter for Low Salinity Flooding-The Relative Importance of Crude Oil, Brine and Rock." In *IOR 2013-17th European Symposium on Improved Oil Recovery*. 2013.

Bond Products and imbibition measurements





From: Eftekhari, A. A., H. Baghooee, M. la Cour Christensen, K. Thomsen, H. M. Nick, and E. Stenby. "Uncertainties in the Mechanistic Models of the Modified Brine Water-flooding of Chalk." In *IOR 2017-19th European Symposium on Improved Oil Recovery*. 2017.

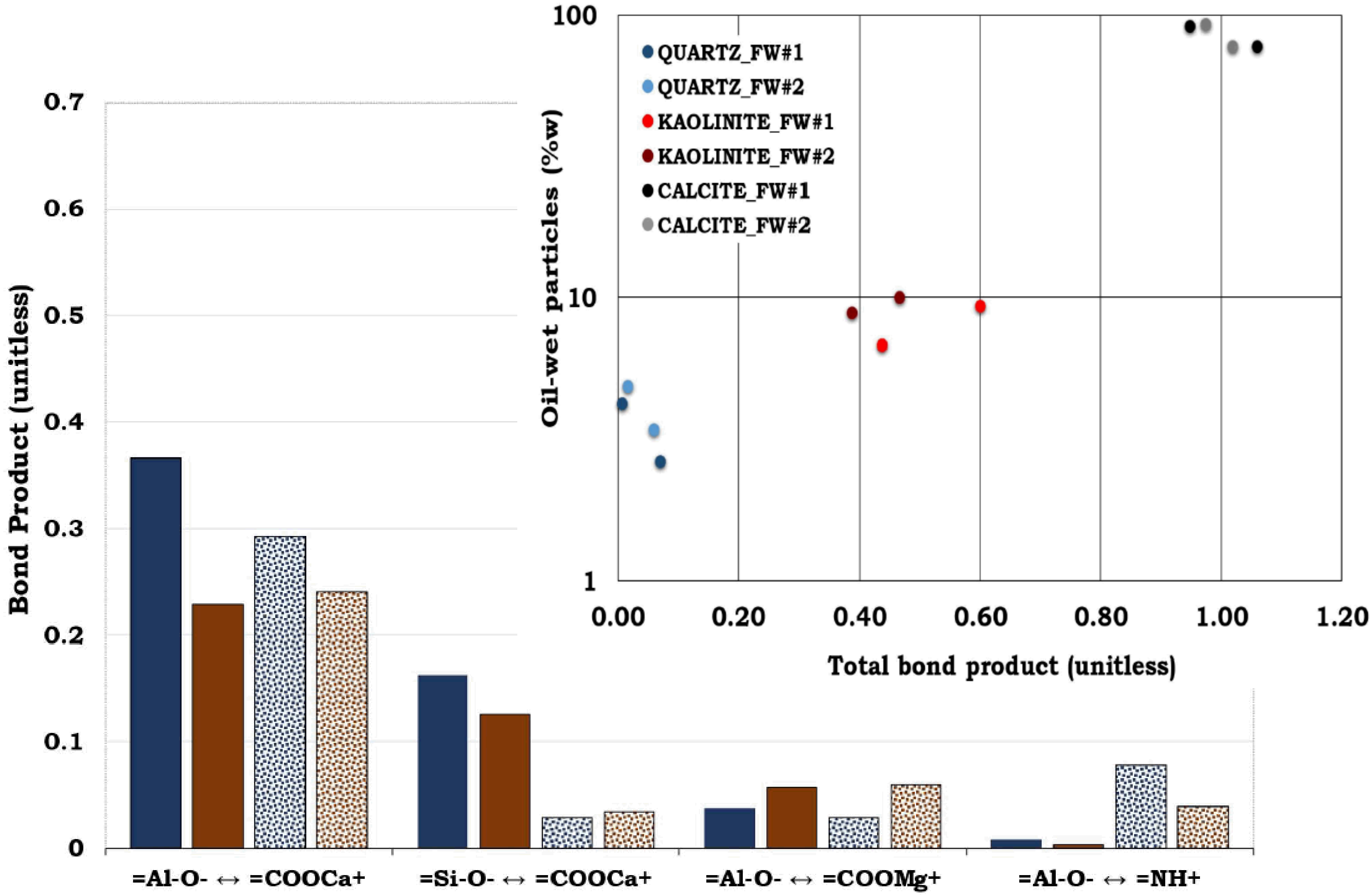


Figure 3—The bond product of the dominant electrostatic pair linkage in kaolinite

From: Erzuah, S., I. Fjelde, and A. V. Omekeh. "Wettability Estimation by Surface Complexation Simulations." In *79th EAGE Conference and Exhibition 2017-SPE EUROPEC*. 2017.

Bond Products and Core floods

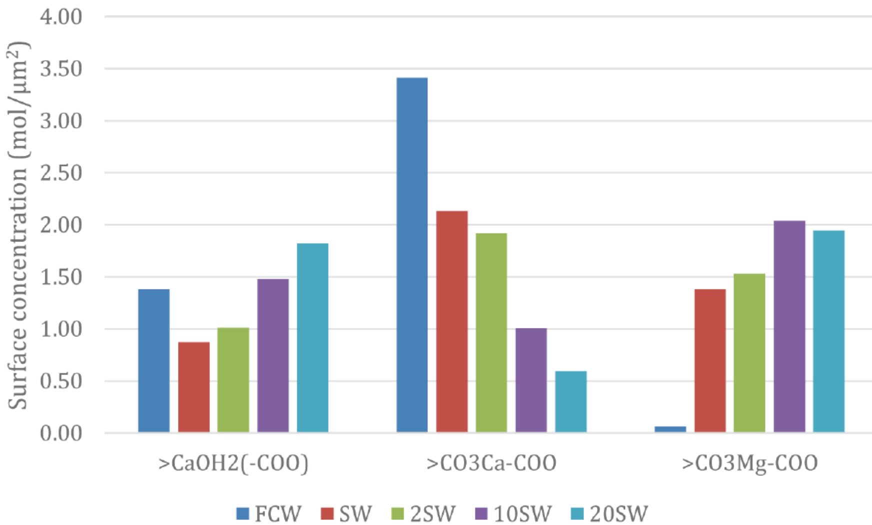
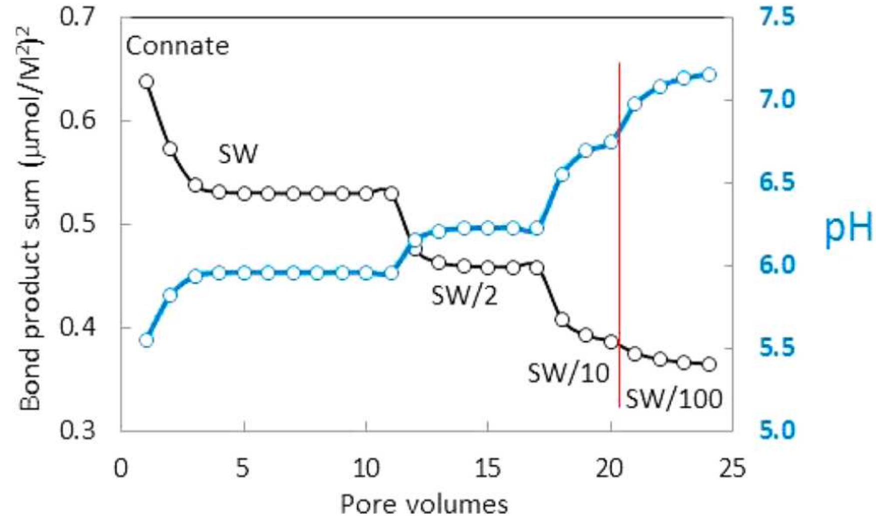
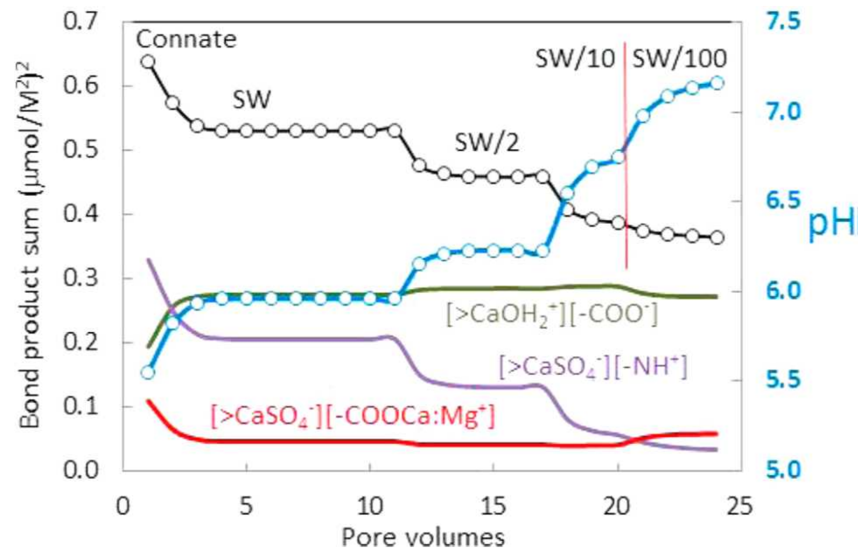


Figure 2—Calculated adsorbed carboxylic acid for brine in Yousef et al. (2010).

From: Qiao, Changhe, Li Li, Russell T. Johns, and Jinchao Xu. "A mechanistic model for wettability alteration by chemically tuned waterflooding in carbonate reservoirs." *SPE Journal* 20, no. 04 (2015): 767-783.

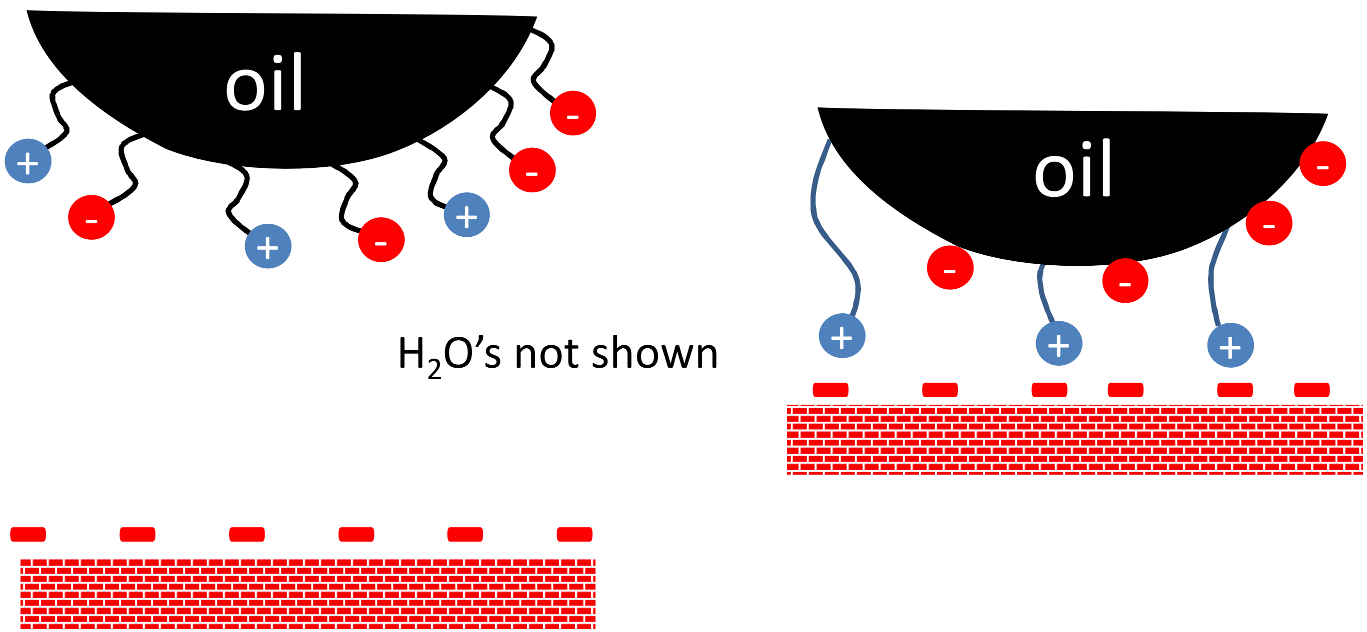




Brady, Patrick V., and Geoffrey Thyne. "Functional wettability in carbonate reservoirs." *Energy & Fuels* 30, no. 11 (2016): 9217-9225.

Oil Surface Chemistry Peculiarities

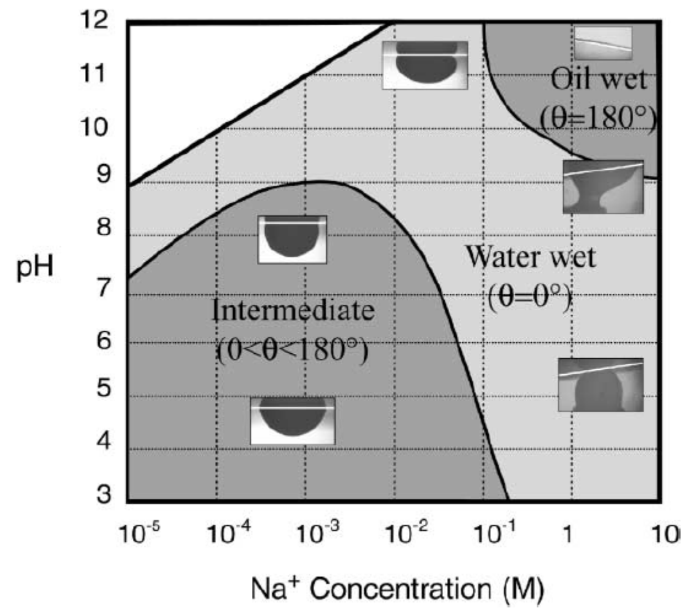
1. Smudged pK_a's,
2. Self-association of acids and bases,
3. Other surface groups,
4. "Hairiness".



After Somasundaran et al., 1993 "Role of reconformation of hairs in anomalous deposition of zwitterionic latex particles." *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 142, no. 1: 83-89.

Hairy DLVO

Drummond and Israelachivilli (2004) “It is important to emphasize that the results obtained with this crude oil cannot be explained in terms of the DLVO theory alone, and it is necessary to invoke polymer-like steric and bridging interactions, to quantitatively describe the measured force profiles”



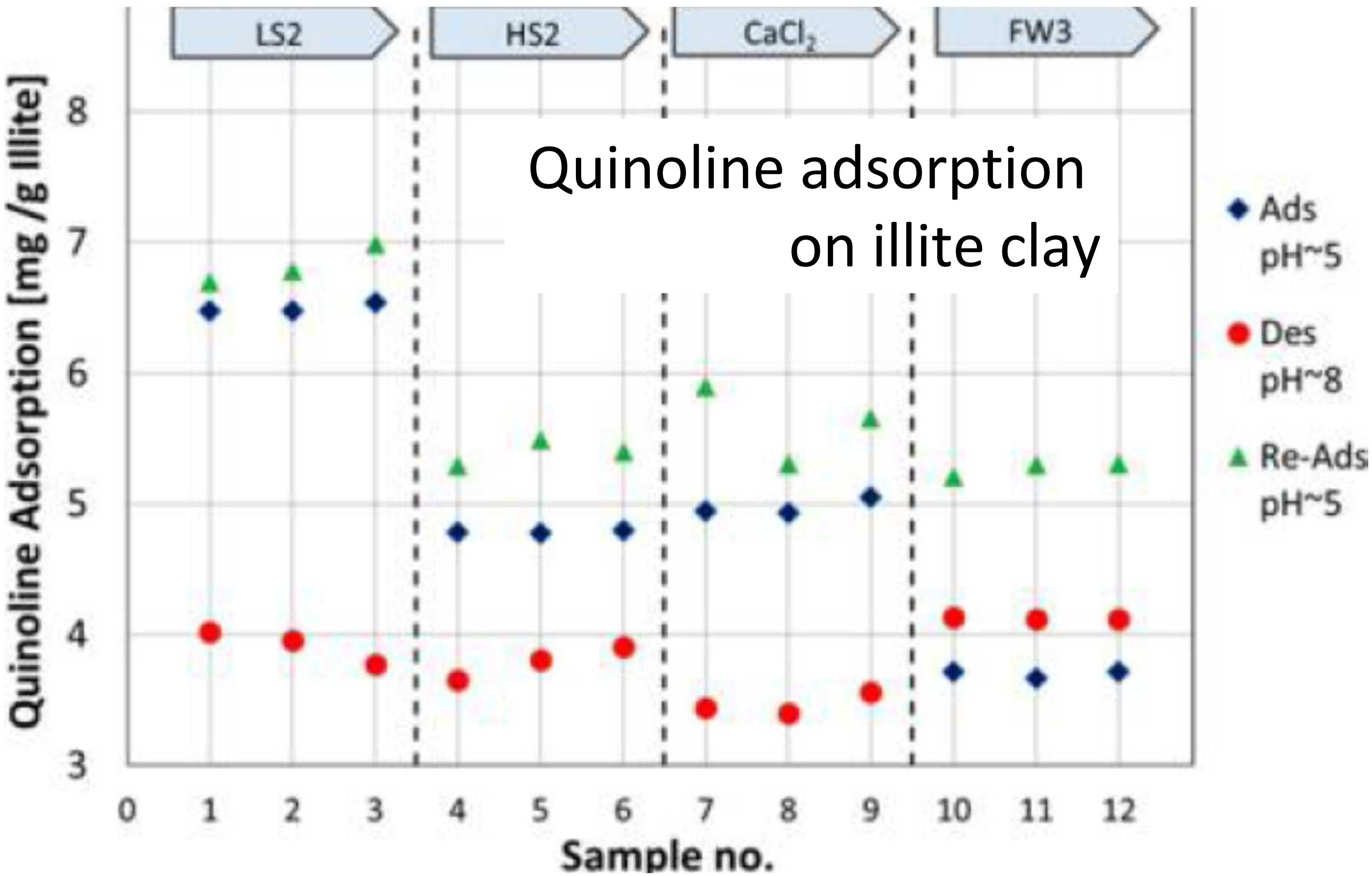
Drummond, Carlos, and Jacob Israelachvili. "Fundamental studies of crude oil–surface water interactions and its relationship to reservoir wettability." *Journal of Petroleum Science and Engineering* 45, no. 1 (2004): 61-81.

From Somasundaran et al. 1998, Role of reconformation of hairs in anomalous deposition of zwitterionic latex particles. Colloids and Surfaces.

5. Unconventional deposition of zwitterionic latex particles

It is proposed that the deposition of the zwitterionic latex particles to be due to the rearrangement of the mixed charge groups present in the latex surface in such a manner that the positive charge sites are extended towards the glass surface and the negative ones retracted away from it. Thus even though the overall average zeta potential is negative, the hairy charges are proposed to reconfigure when the two surfaces begin to feel each other.

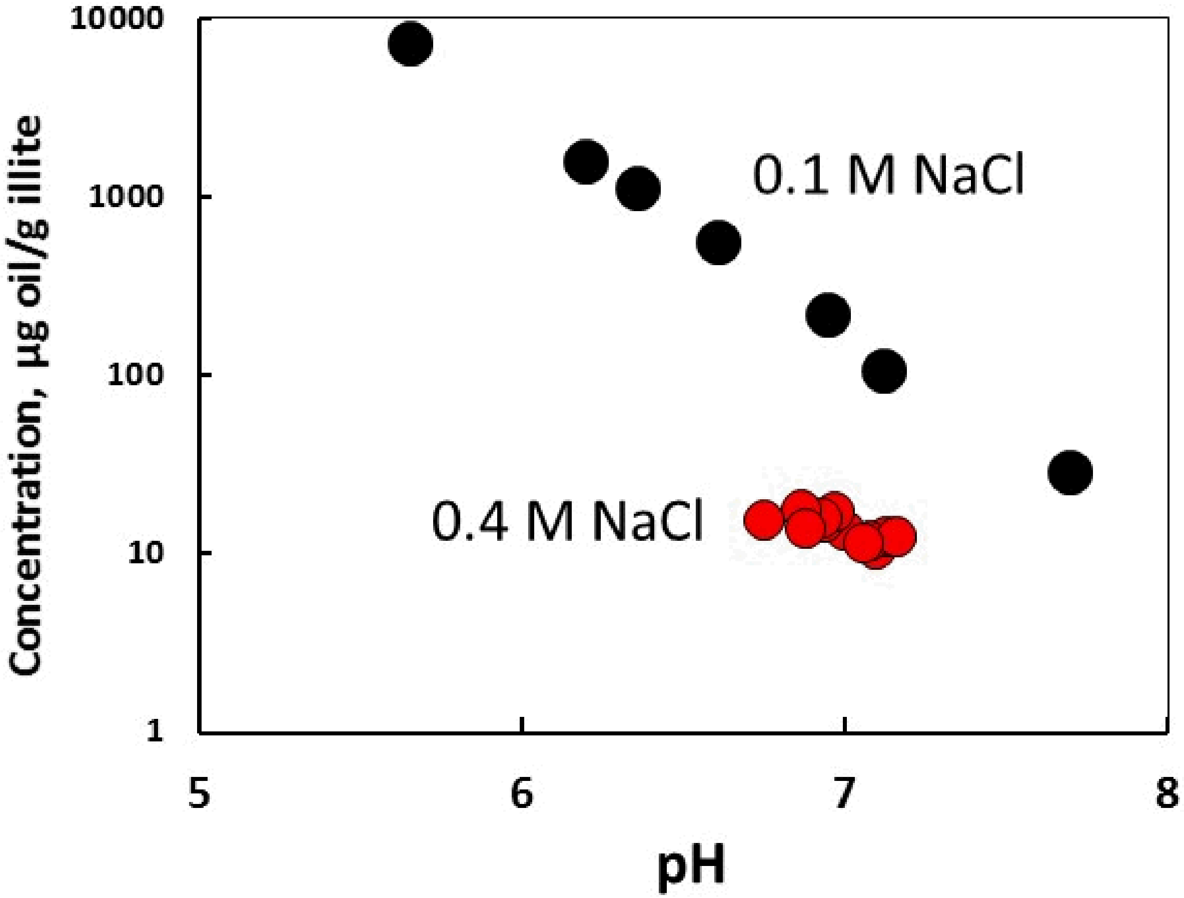
Zeta Potentials tell only a small part of the story



From: Aghaeifar, Zahra, Skule Strand, Tor Austad, Tina Puntervold, Hakan Aksulu, Kine Navratil, Silje Storås, and Dagny Håmsø. "Influence of Formation Water Salinity/Composition on the Low-Salinity Enhanced Oil Recovery Effect in High-Temperature Sandstone Reservoirs." *Energy & Fuels* 29, no. 8 (2015): 4747-4754.

Oil Adsorption on Illite

Source: C.R. Bryan, Sandia Labs



Both Oil and Illite have negative zeta potentials, but there is still sorption.

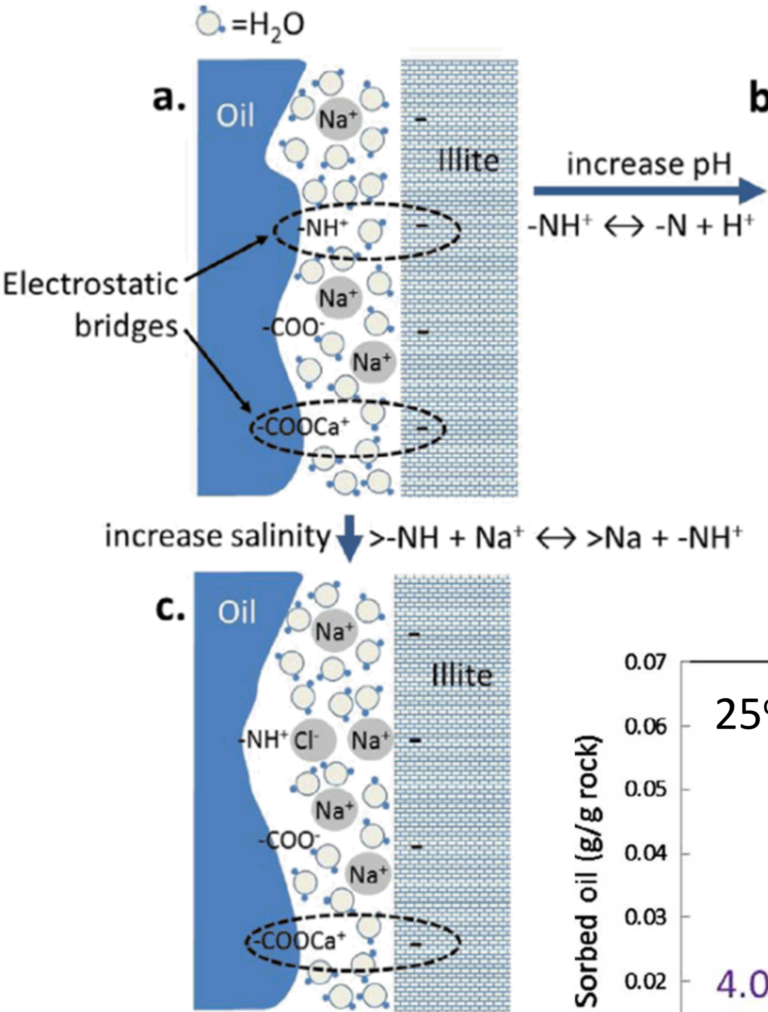
Decreased ionic strength thickens the double layer, but increases oil sorption.

Something besides classical DLVO is controlling wettability.

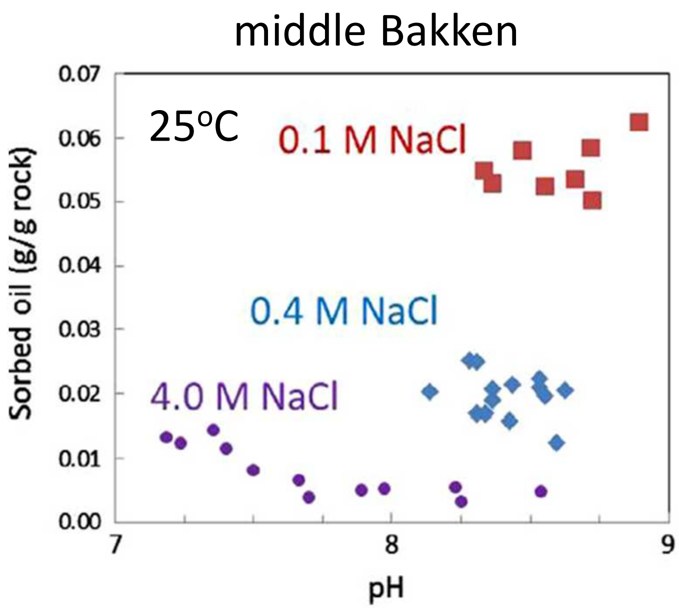
Oil from West Pearl Queen Field, Hobbs, New Mexico

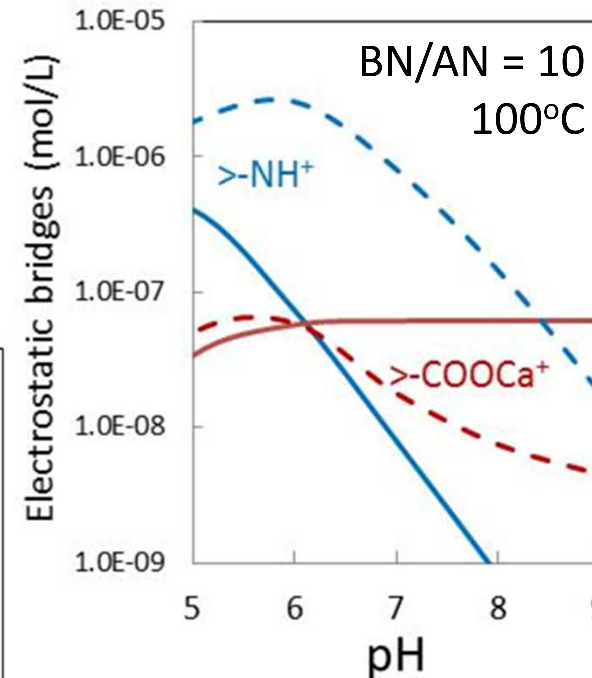
TBN/TAN ~ 1.3

Oil Adhesion to Tight Formations (Illite)



Brady et al. (2016) J. Unconventional Oil and Gas Resources

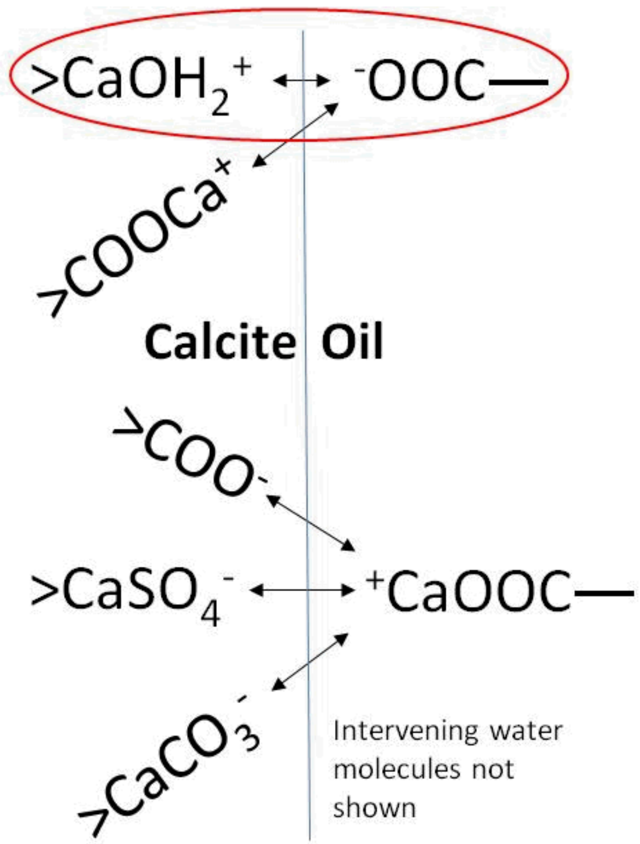


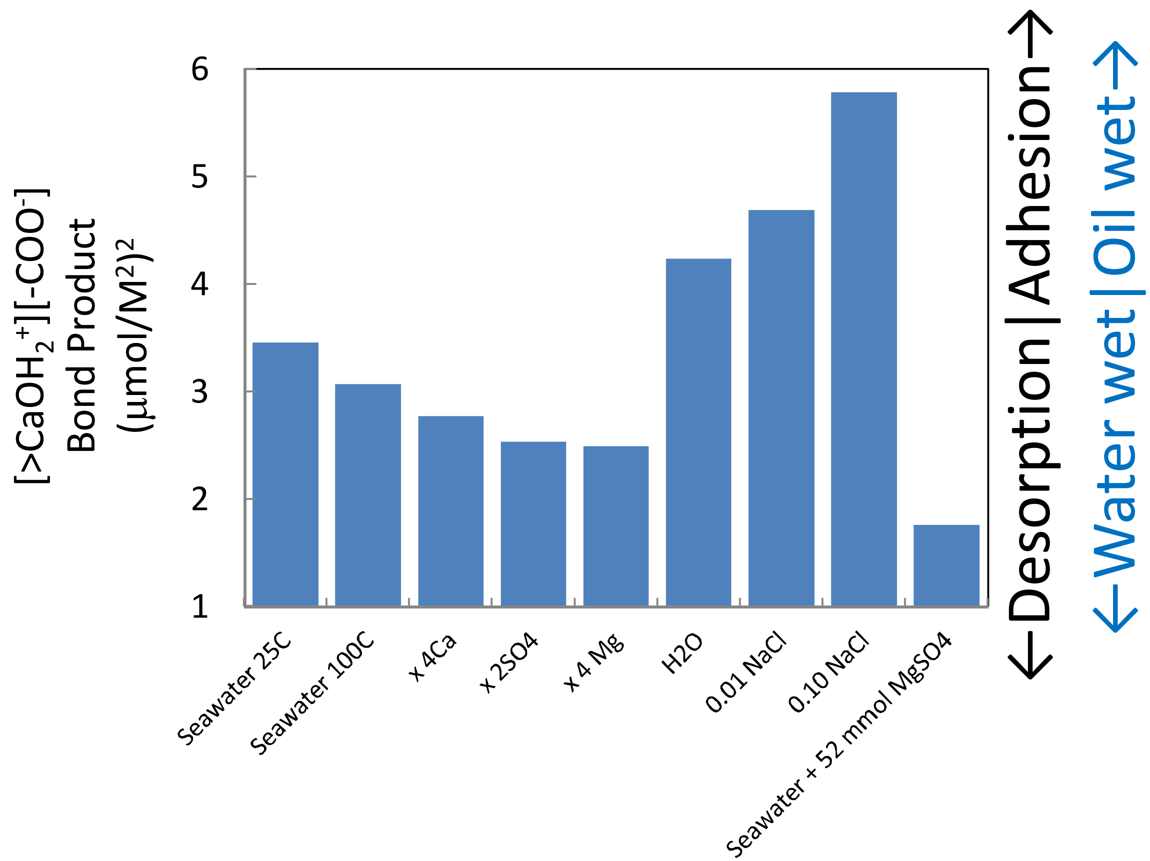


Basin	Production (mbbl/d)	% Carbonate	% Clay	% Kerogen	Dominant clay
Permian	2040	5–40	10–40	1–10	Illite
Bakken	1220	10–15	10–20	2–8	Illite
Eagle Ford	900	40–60	10–40	5–10	Smec/illite/kaol

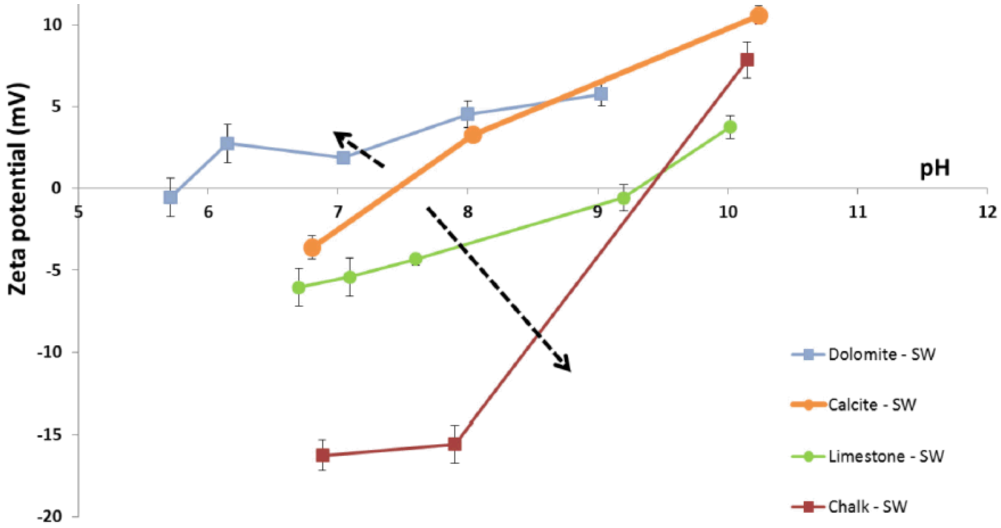
[a] Balance is mostly quartz or biogenic silica.

Oil-Limestone Adhesion

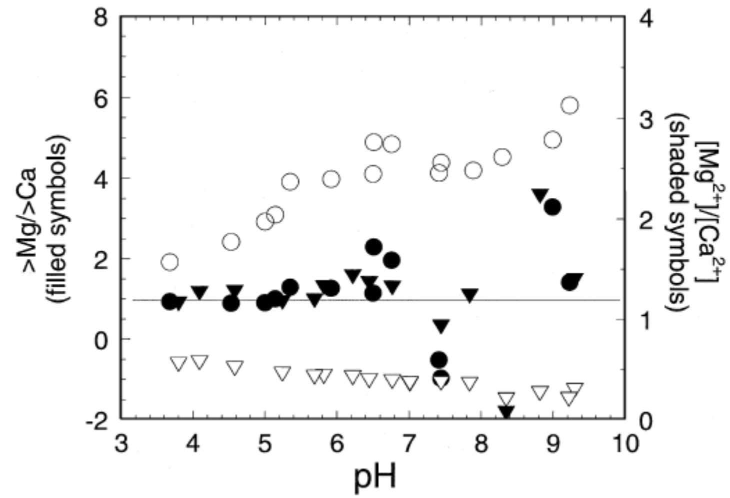




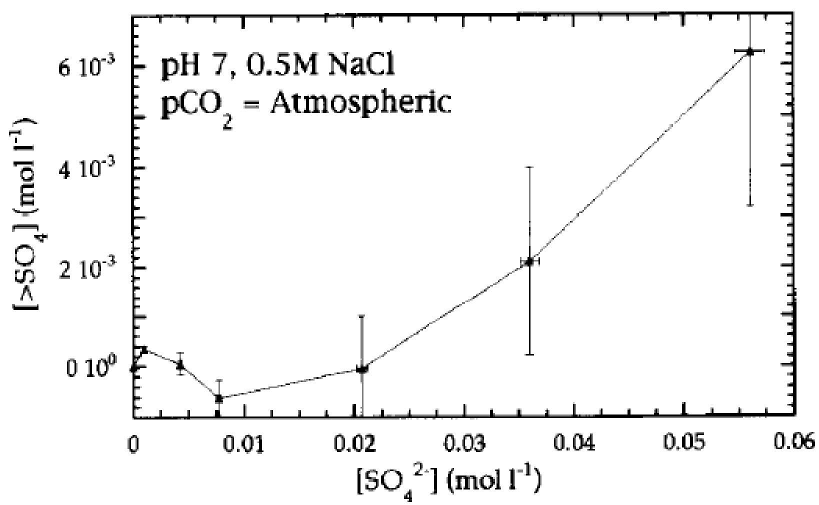
From: Brady, Patrick Vane, James L. Krumhansl, and Paul E. Mariner. "Surface complexation modeling for improved oil recovery." In *SPE Improved Oil Recovery Symposium*. Society of Petroleum Engineers, 2012.



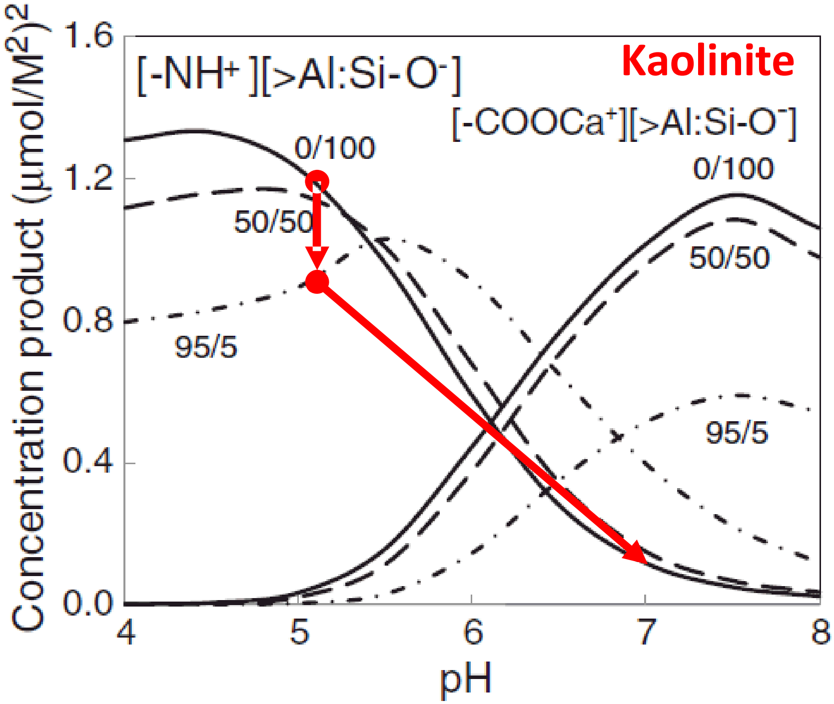
From: Mahani, Hassan, Arsene Levy Keya, Steffen Berg, and Ramez Nasralla. "Electrokinetics of carbonate/brine interface in low-salinity waterflooding: Effect of brine salinity, composition, rock type, and pH on ζ-potential and a surface-complexation model." *SPE Journal* (2016).

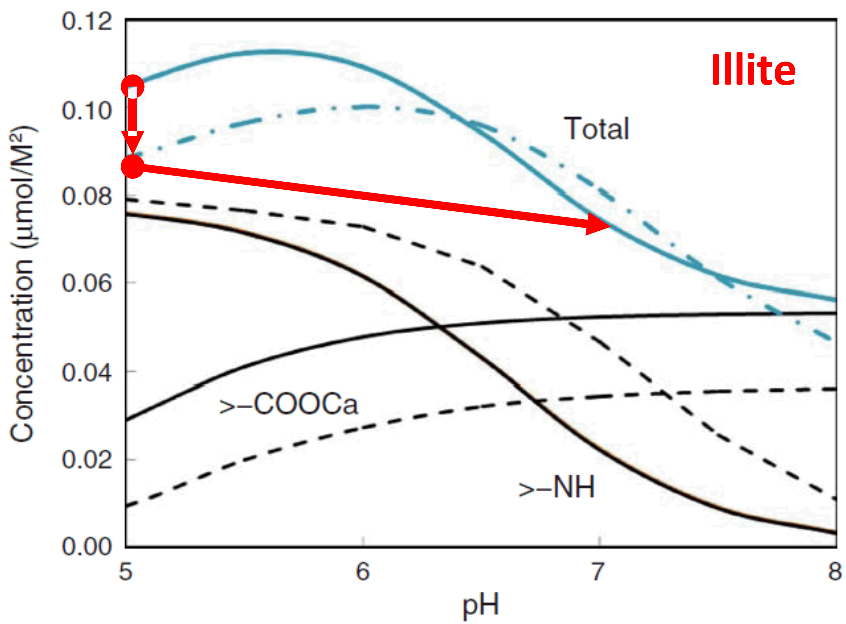


Brady, Patrick V., Hans W. Papenguth, and John W. Kelly. "Metal sorption to dolomite surfaces." *Applied Geochemistry* 14, no. 5 (1999): 569-579.

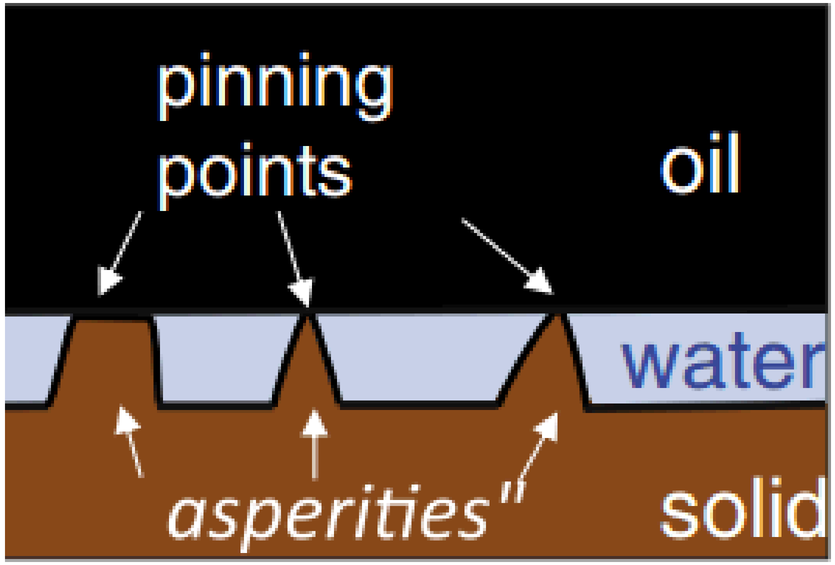


Brady, Patrick V., James L. Krumhansl, and Hans W. Papenguth. "Surface complexation clues to dolomite growth." *Geochimica et Cosmochimica Acta* 60, no. 4 (1996): 727-731.

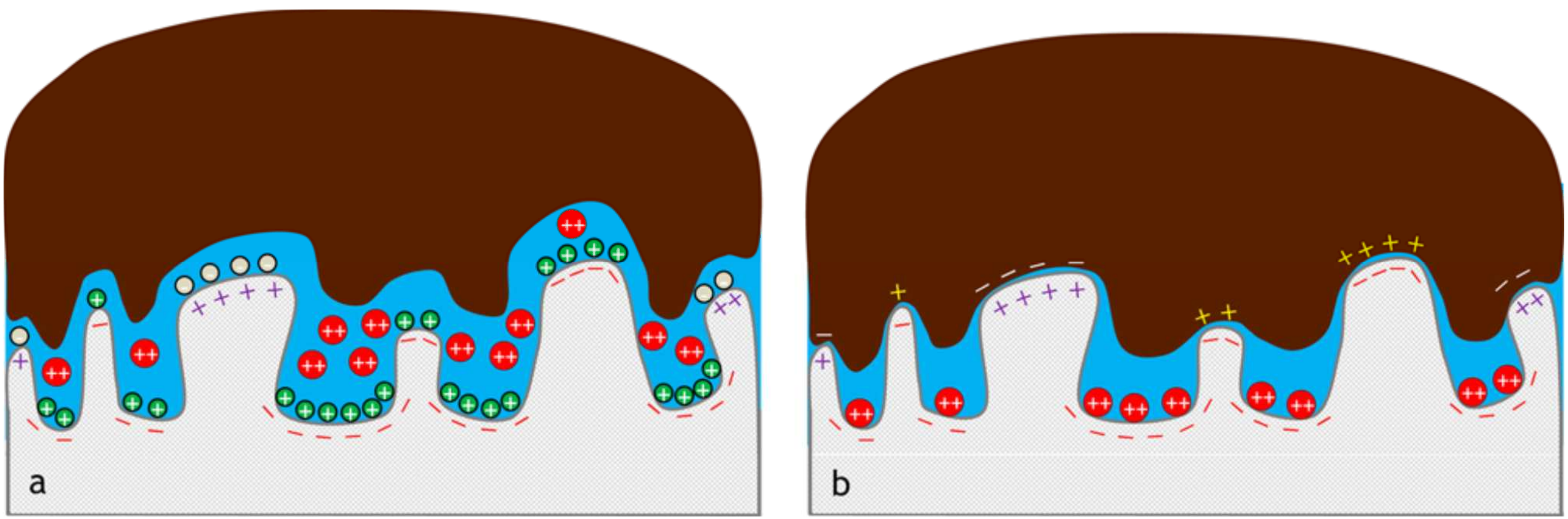




Decreasing salinity increases pH which (usually) decreases the bond product, which usually makes more water wet, which usually means more oil.



Schmatz, Joyce, Janos L. Urai, Steffen Berg, and Holger Ott. "Nanoscale imaging of pore-scale fluid-fluid-solid contacts in sandstone." *Geophysical Research Letters* 42, no. 7 (2015): 2189-2195.



From: Farajzadeh, Rouhi, Hua Guo, Julia van Winden, and J. Bruining. "Cation exchange in the presence of oil in porous media." *ACS Earth and Space Chemistry* (2017).

Sandstone + Kaolinite + Calcite Cement at 60°C