Altering Wettability, Designing Anti-viral Drugs, and Preventing Potholes

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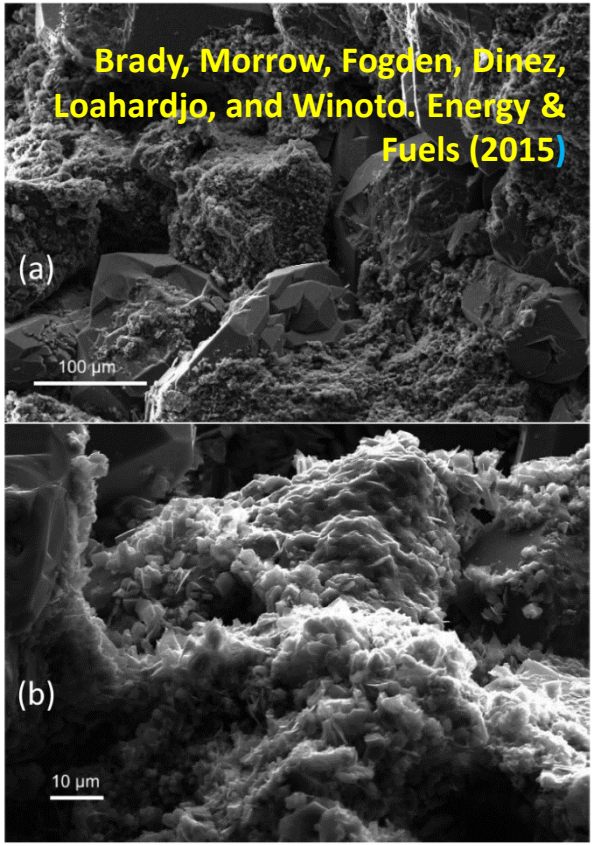
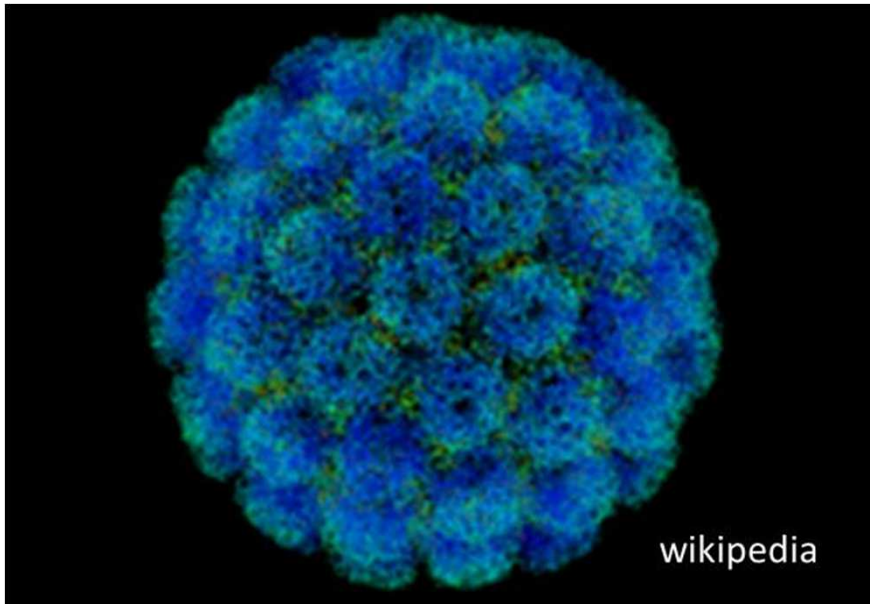
SAND2017-10195C





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

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… in the April 30, 2016 issue of The Economist

The Economist | World politics | Business & finance | Economics | Science & technology | Culture | Blogs | Debate | Multimedia | Print edition

Viral infections

General knowledge

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Progress towards a broad antiviral treatment

Apr 30th 2016 | From the print edition

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… 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

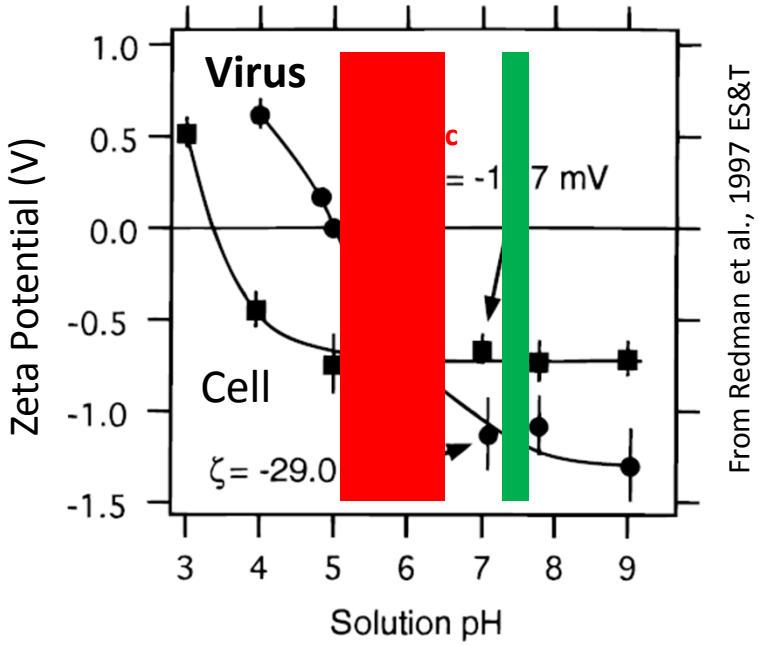
General knowledge

Buddy, can you spare a

Follow *The*

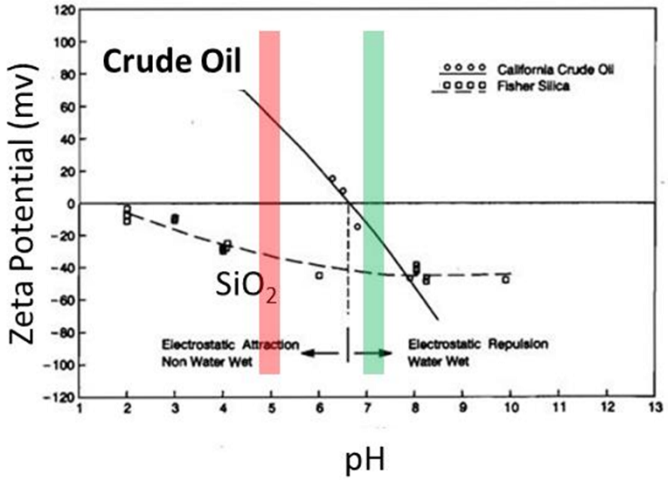
Endosomal pH 5-6.5 Blood plasma pH 7.4

Virus on Cell

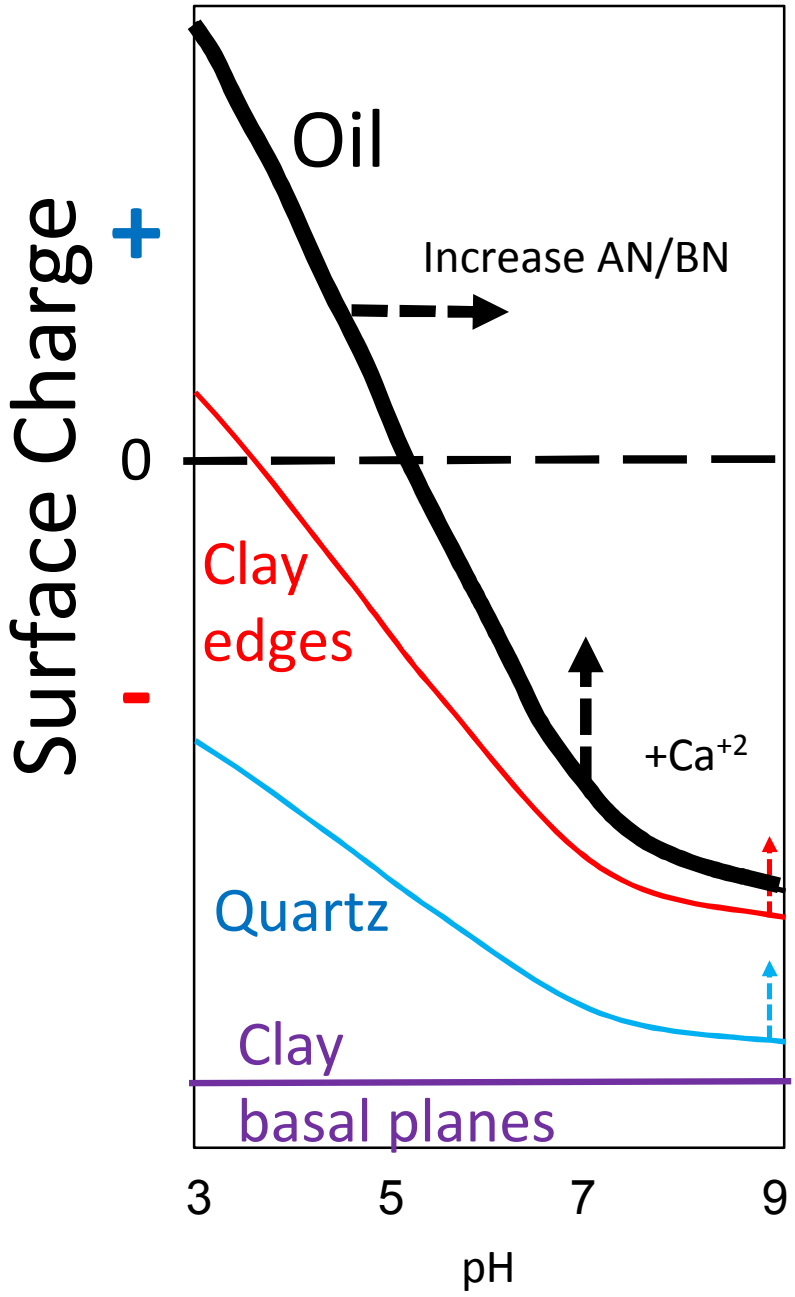


From Redman et al., 1997 ES&T

Oil on Rock



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



Oil

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

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

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

Clay Edges

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

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

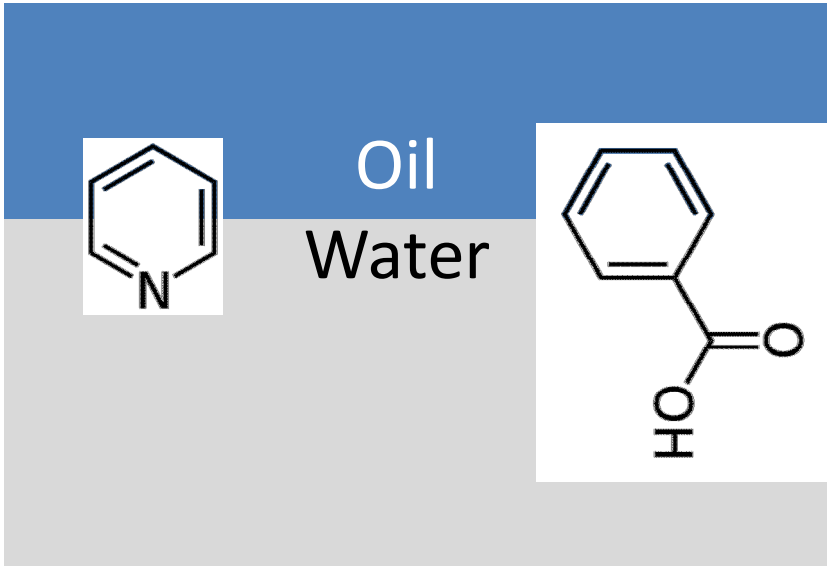
Quartz

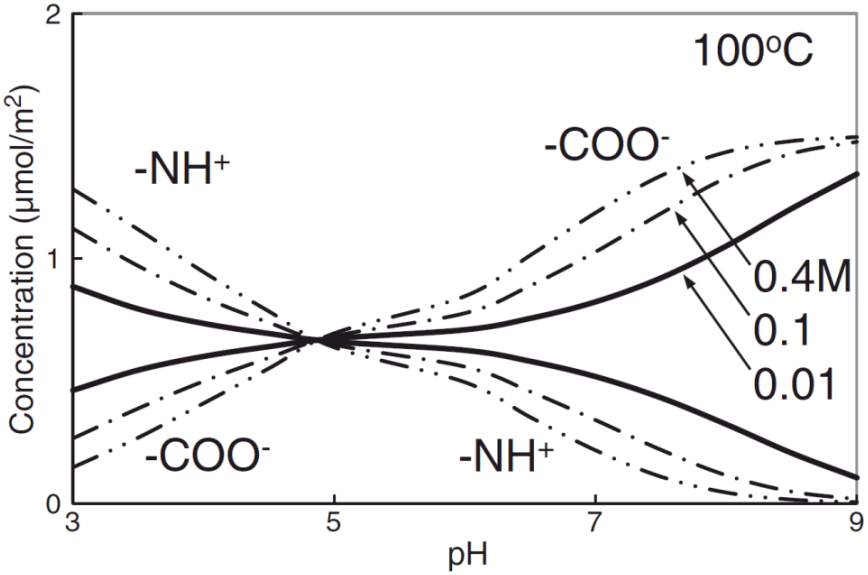
$>Si\text{-}O\text{-}H \leftrightarrow >Si\text{-}O^- + H^+$

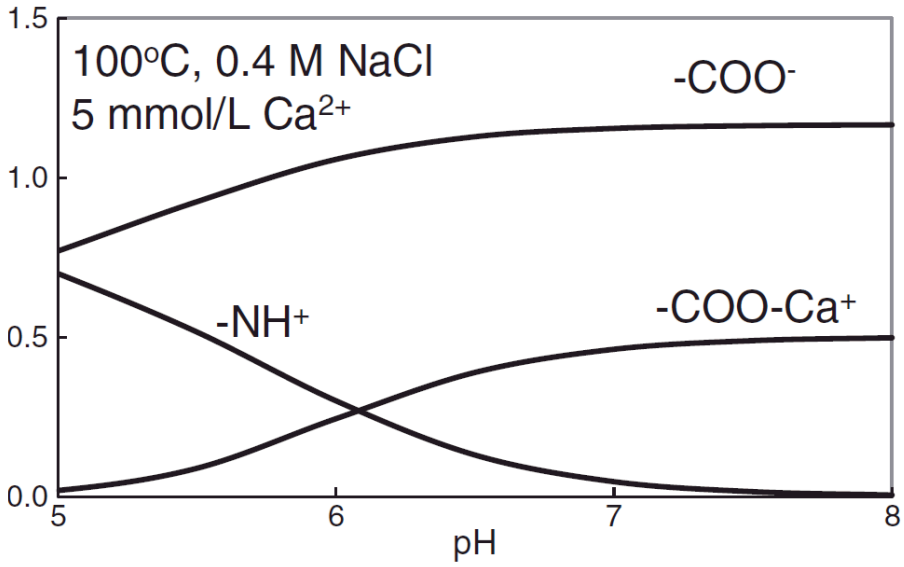
Clay Basal Planes

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

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



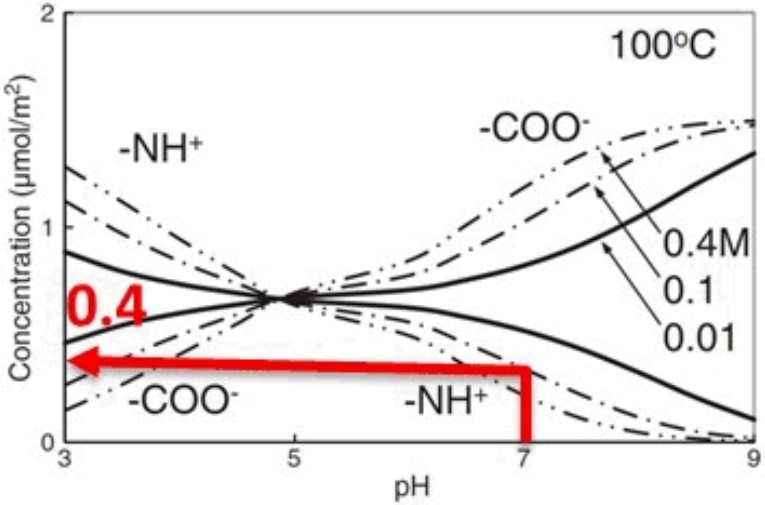




From: Brady, Patrick V., and James L. Krumhansl. "A surface complexation model of oil–brine–sandstone interfaces at 100° C: Low salinity waterflooding." *Journal of Petroleum Science and Engineering* 81 (2012): 171-176.

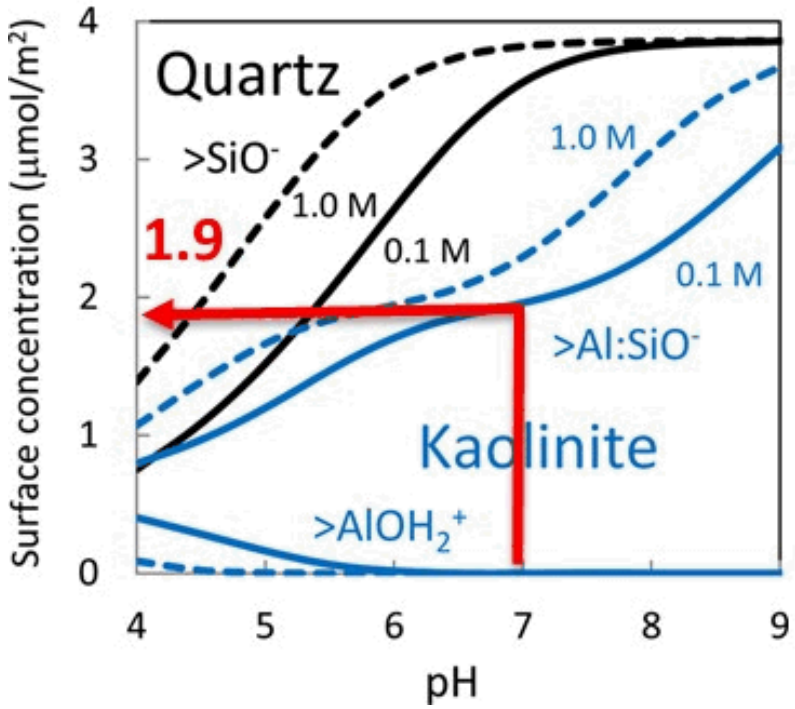
How to Model Oil-Rock Adhesion?

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

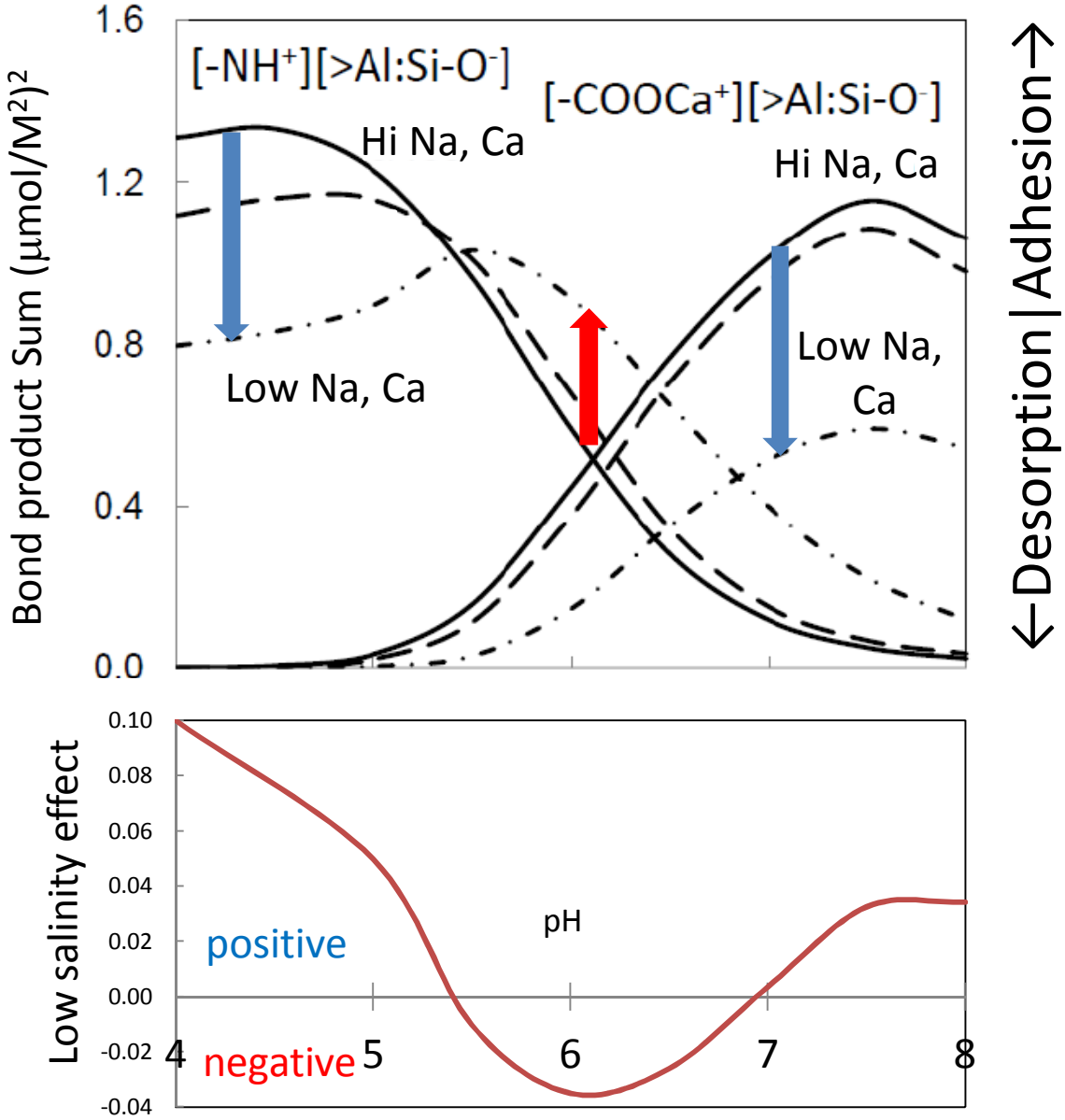


Example: Oil-NH^+ to Kaolinite $>AlO^-$, pH 7, 0.1M NaCl, 100°C.

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.

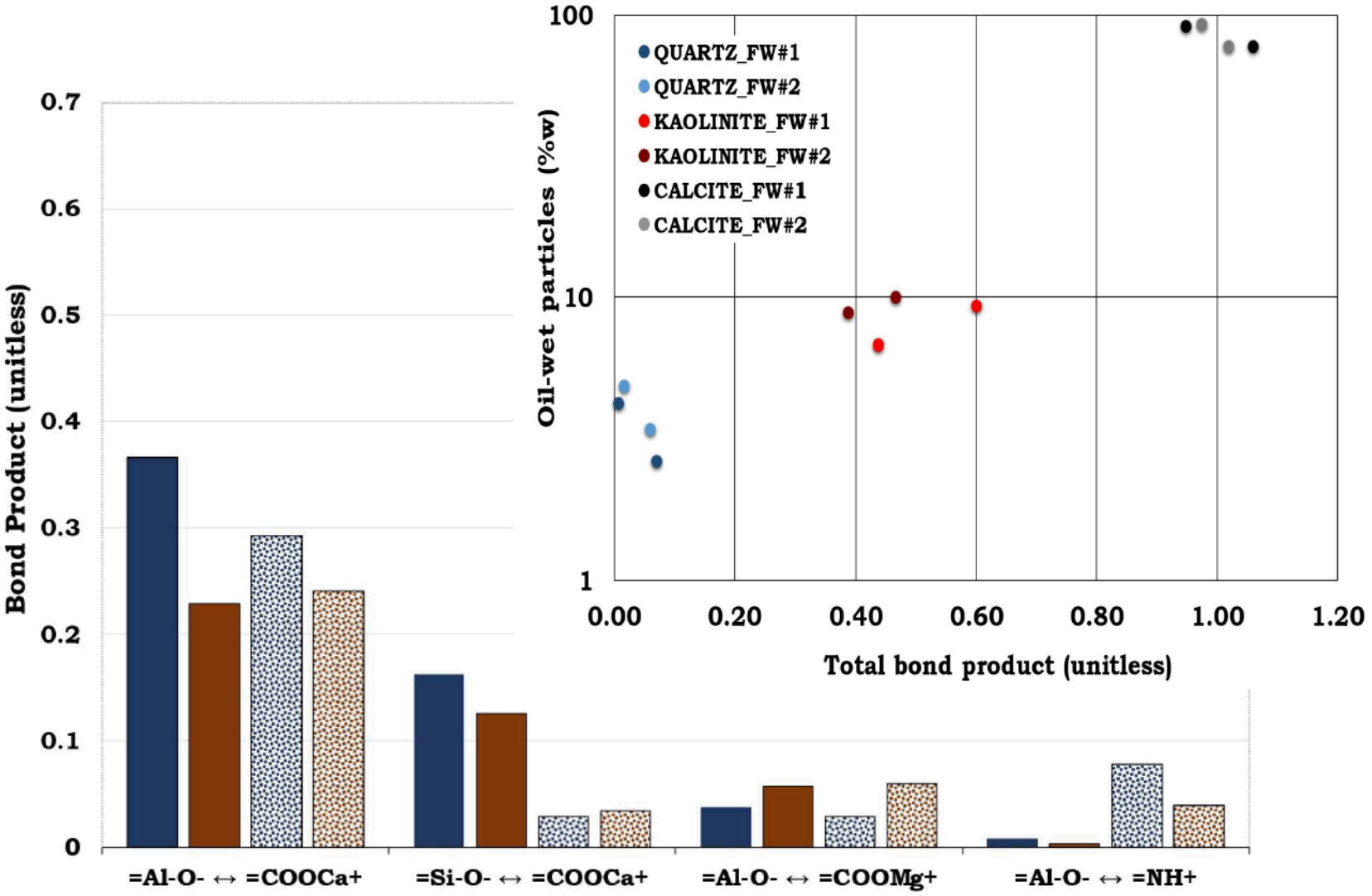
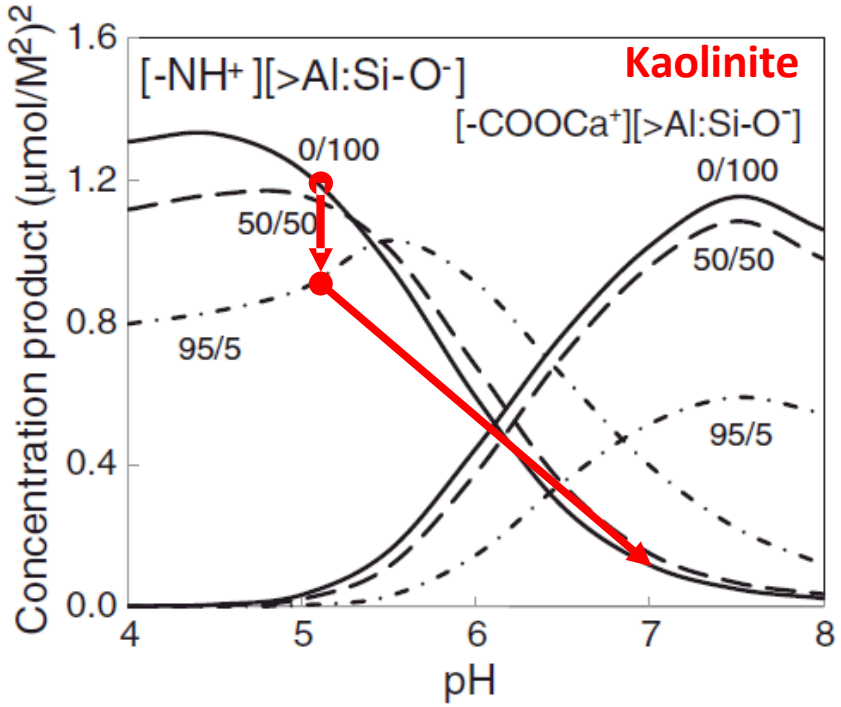
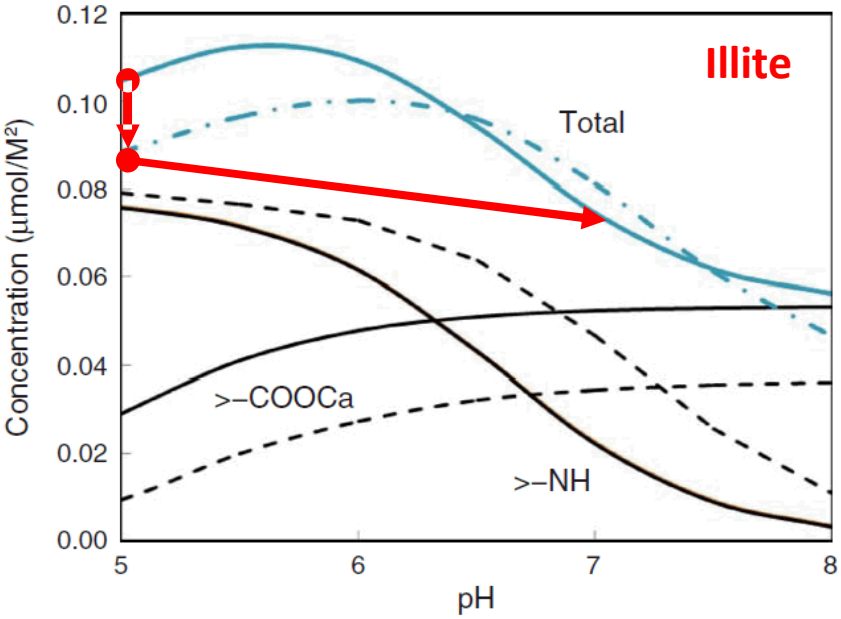


Figure 3—The bond product of the dominant electrostatic pair linkage in kaolinite

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.

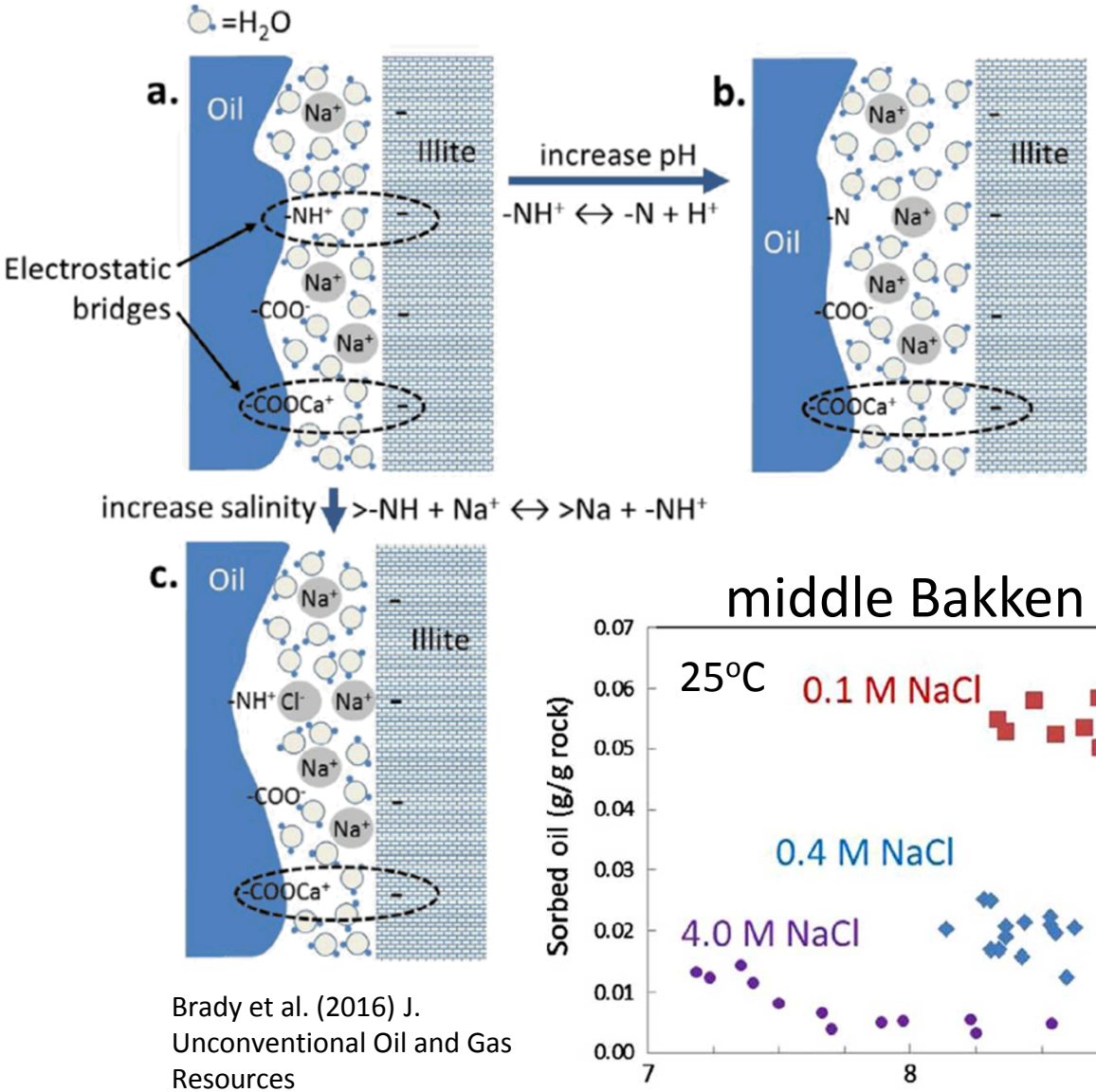




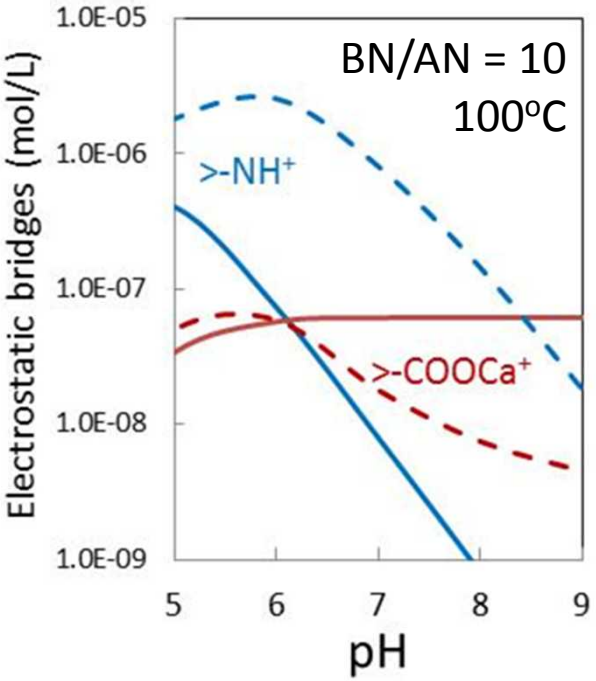
Decreasing salinity increases pH which usually decreases the bond product, which usually makes things more water wet.

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

Shales



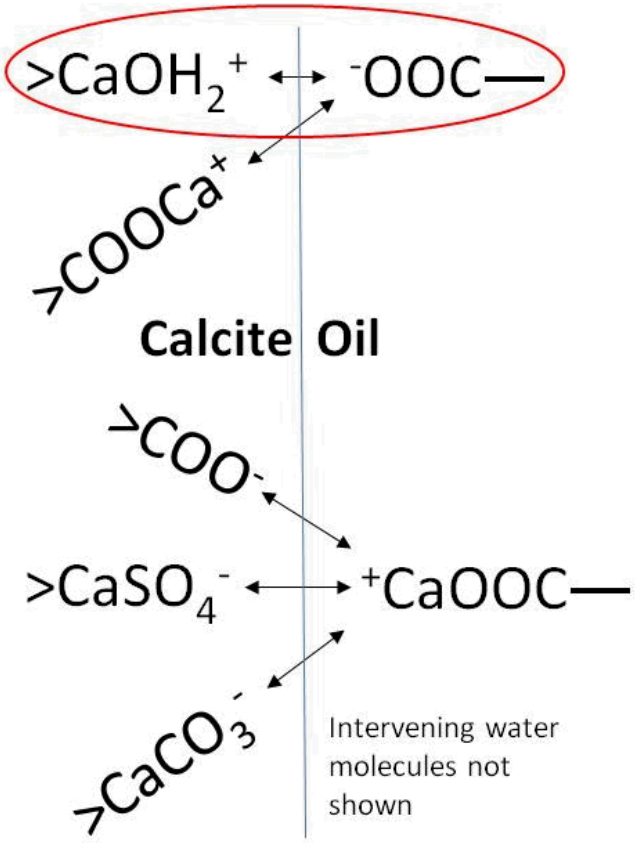
Brady et al. (2016) J. Unconventional Oil and Gas Resources

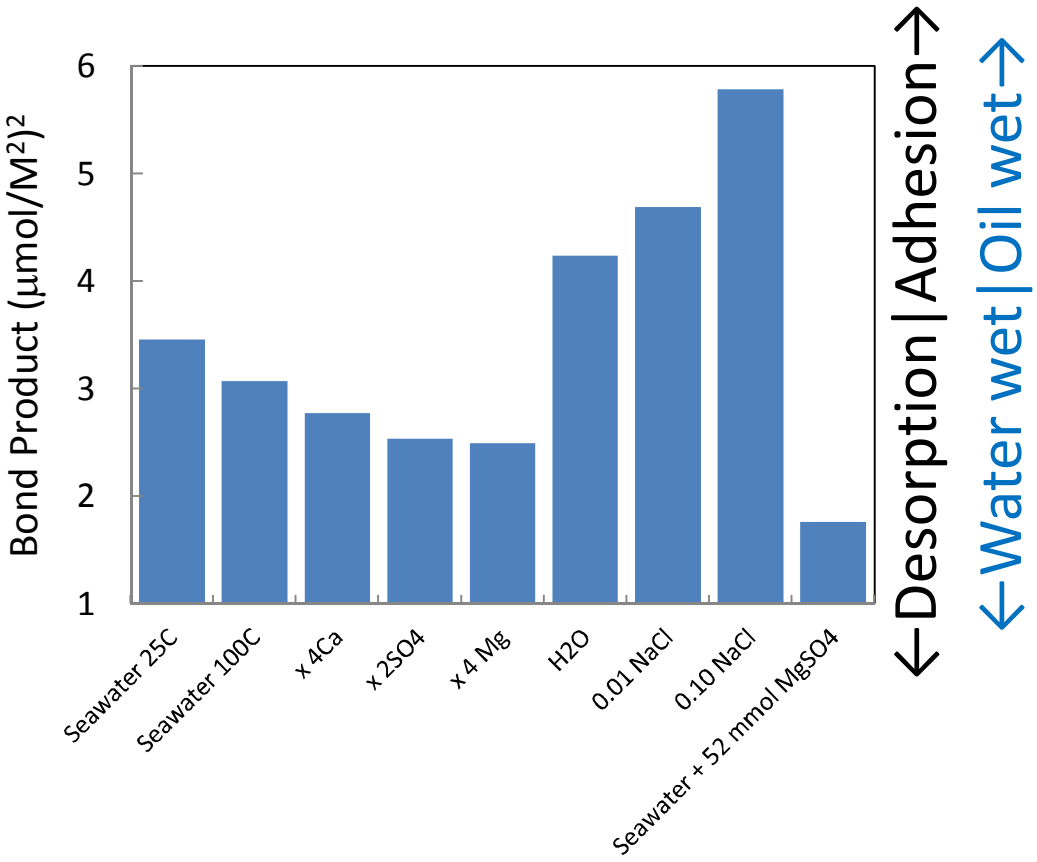


Basin	Production (mbbl/d)	% Carbonate	% Clay	% Kerogen	Dominant clay
Permian	2040	5–40	10–40	1–10	Illite
Bakken	1220	10–15	10–20	2–8	Illite
Eagle Ford	900	40–60	10–40	5–10	Smec/illite/kaol

[a] Balance is mostly quartz or biogenic silica.

Limestones





From: Brady, Patrick V., 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.

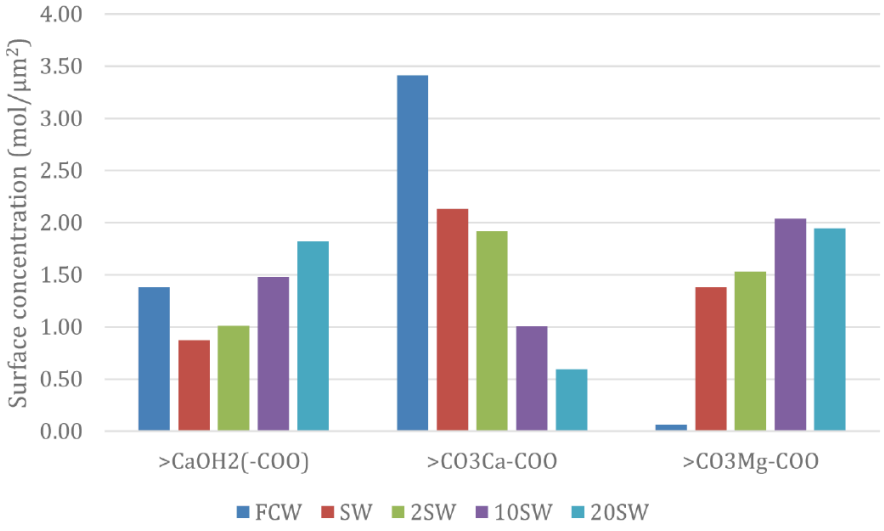
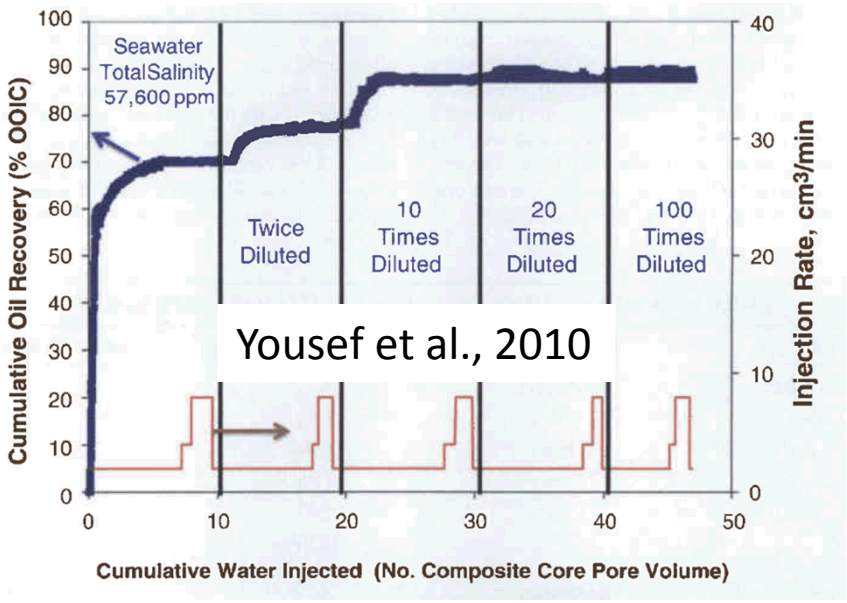
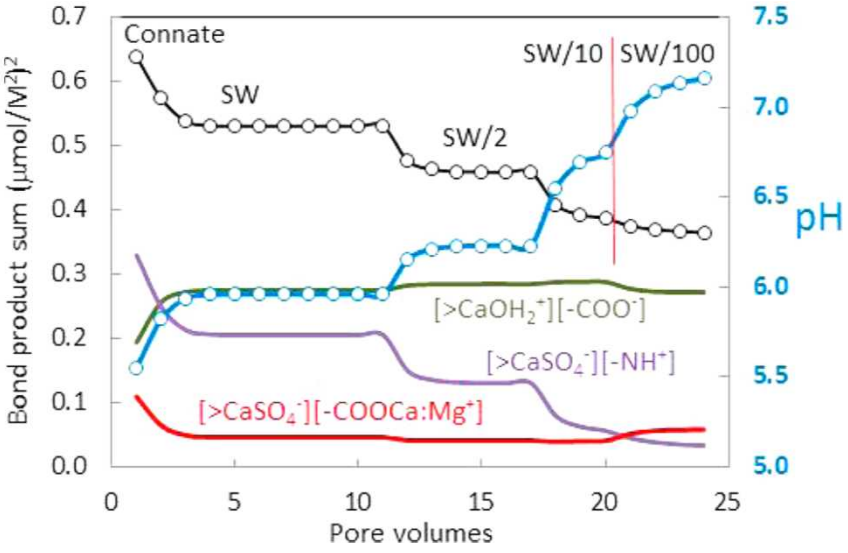


Figure 2—Calculated adsorbed carboxylic acid for brine in Yousef et al. (2010).

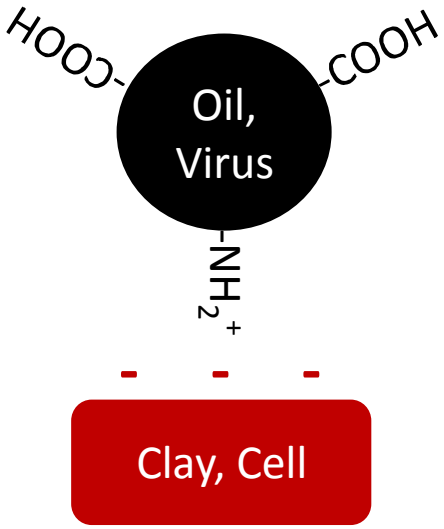
From: Qiao, Changhe, Li Li, Russell T. Johns, and Jinchao Xu. "A mechanistic model for wettability alteration by chemically tuned waterflooding in carbonate reservoirs." *SPE Journal* 20, no. 04 (2015): 767-783.





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

Better drugs; More oil.



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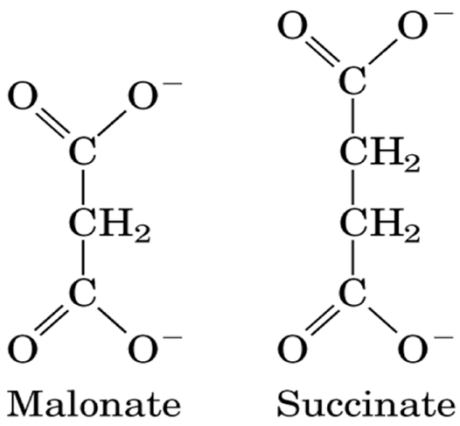

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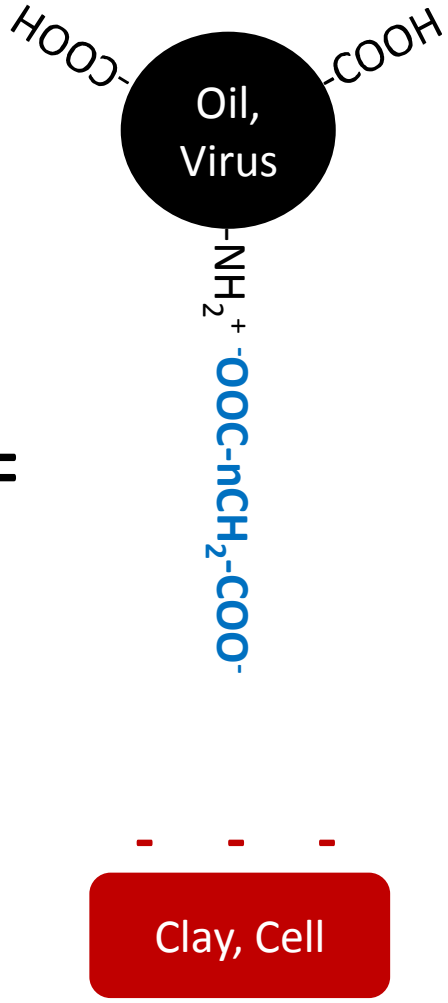


Potential obstacles

More Oil
Solubility w.r.t Ca/Mg
N-Carboxylate binding strength

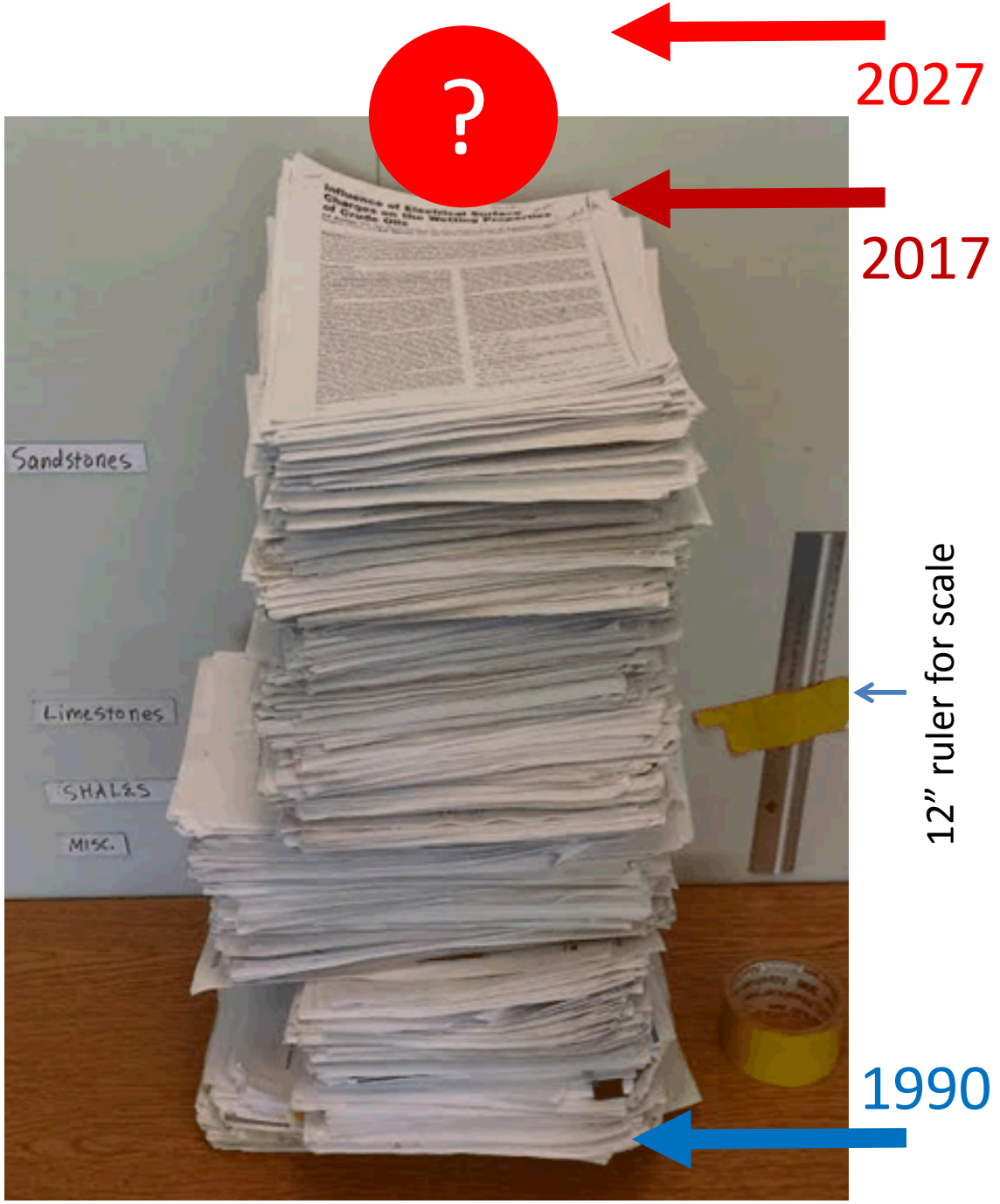
Better Drugs
Speciation in blood plasma,
Linking with proteins,
Toxicity

Oil surface titrations,

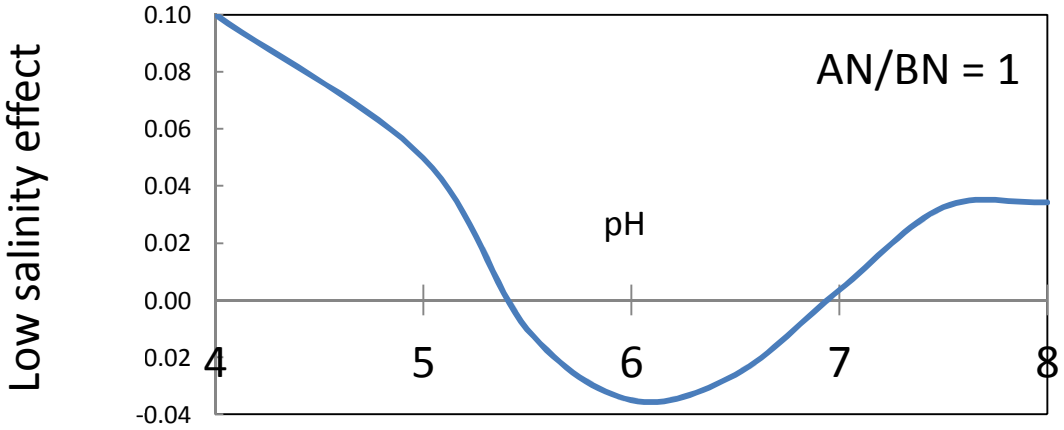
Water wet conditions,

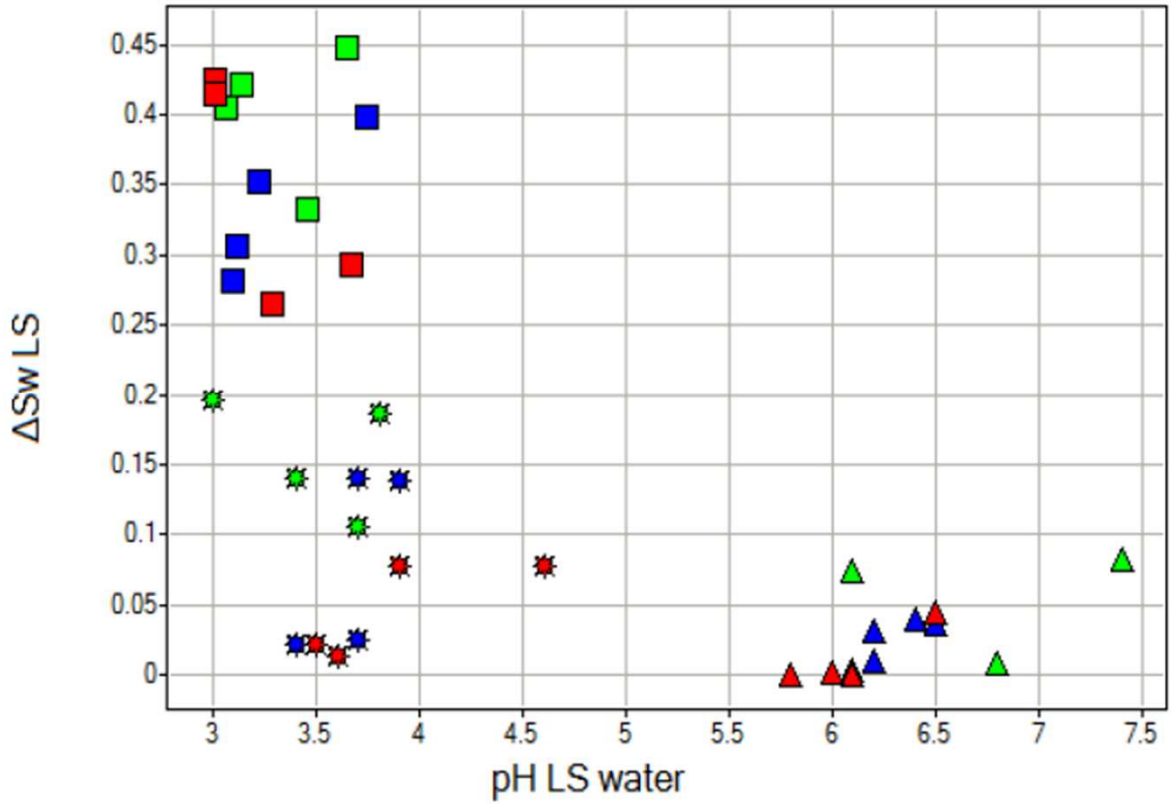
Primary recovery,

Medicine.



Backup Stuff

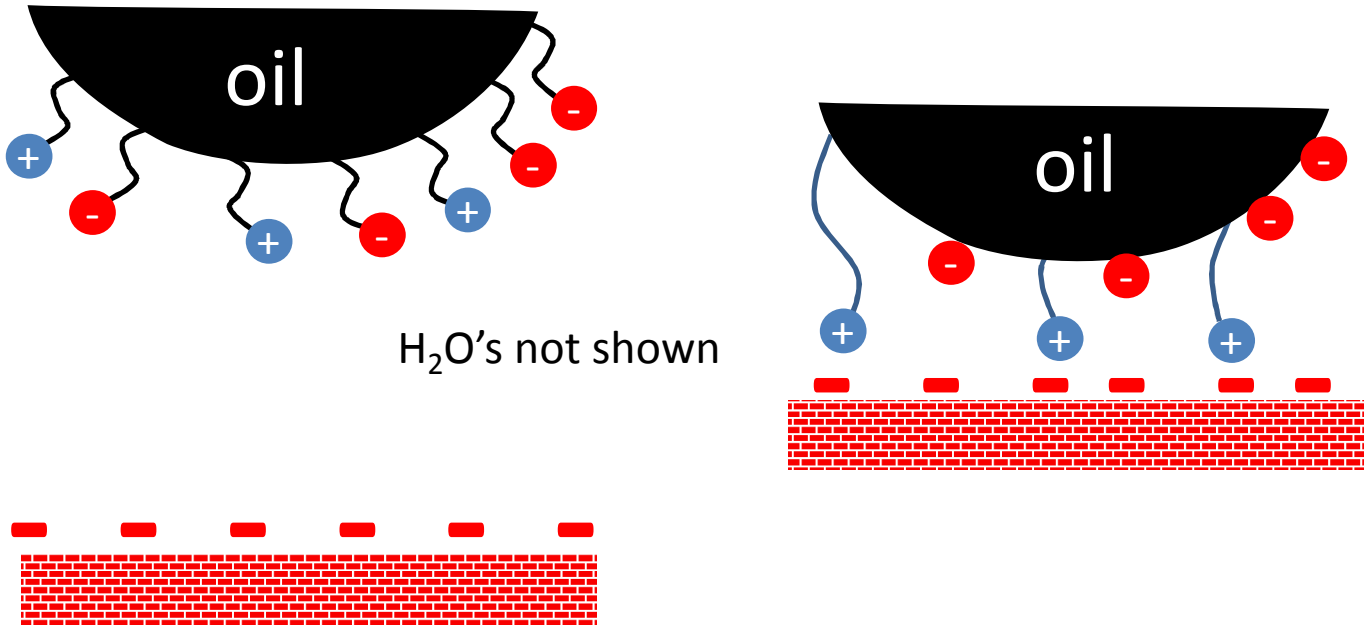




From: Van Winden, J. F., B. M. J. M. Suijkerbuijk, V. Joekar-Niasar, N. J. Brussee, H. A. van der Linde, A. H. M. Marcelis, A. H. Coorn, S. G. J. Pieterse, K. S. Ganga, and I. S. M. Al-Qarshubi. "The Critical Parameter for Low Salinity Flooding-The Relative Importance of Crude Oil, Brine and Rock." In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

Oil Surface Chemistry Peculiarities

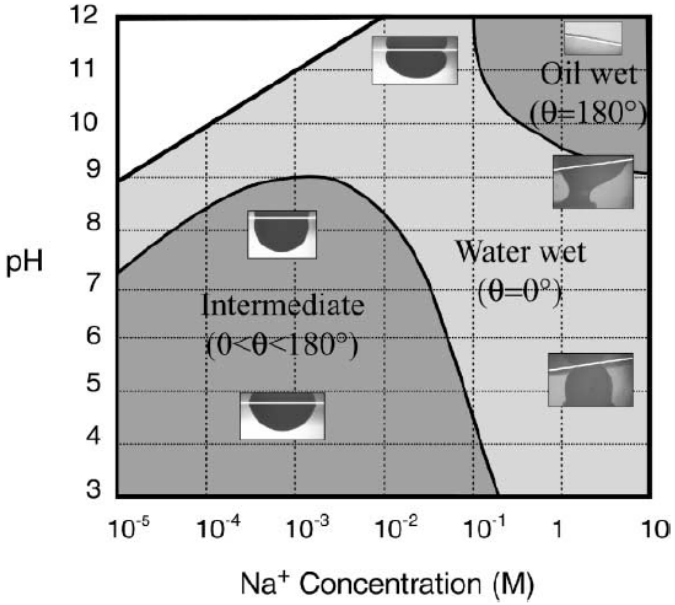
1. Smudged pK_a's,
2. Self-association of acids and bases,
3. Other surface groups,
4. "Hairiness".



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) "… 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.

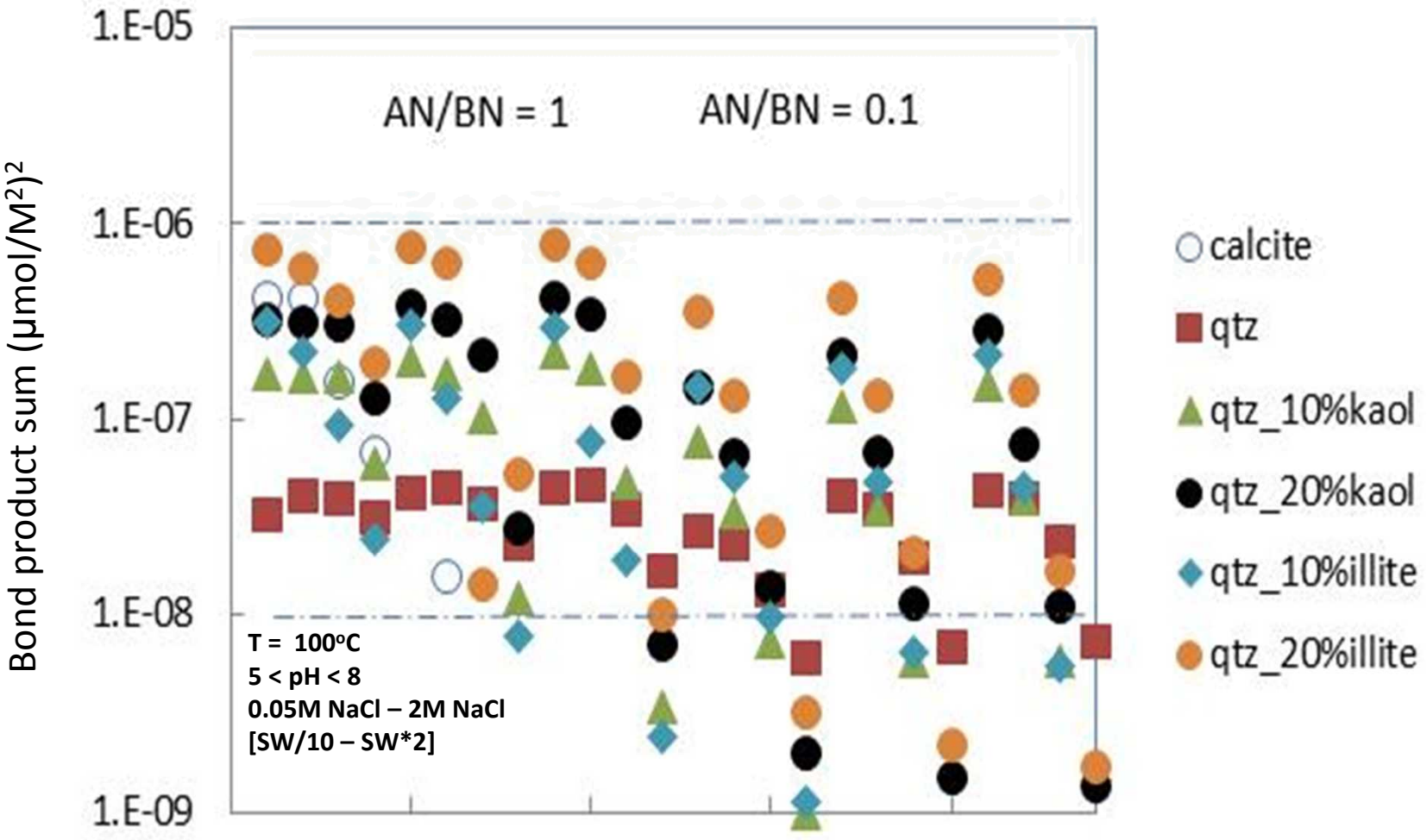
From Somasundaran et al. 1998, Role of reconformation of hairs in anomalous deposition of zwitterionic latex particles. Colloids and Surfaces.

Zeta Potentials are a start …

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.

Initial Wettability and Primary Recovery



Oil Adhesion to the World's Reservoirs

Garrett Gilbert, UT Quarterback in the 2010 BCS Championship Game

Gale Gilbert, Garrett's Dad, Cal Quarterback in the Cal-Stanford Big Game in 1982

In the 1982 Cal-Stanford Big Game with John Elway, all the laterals and the trumpet player in the end zone.

Me