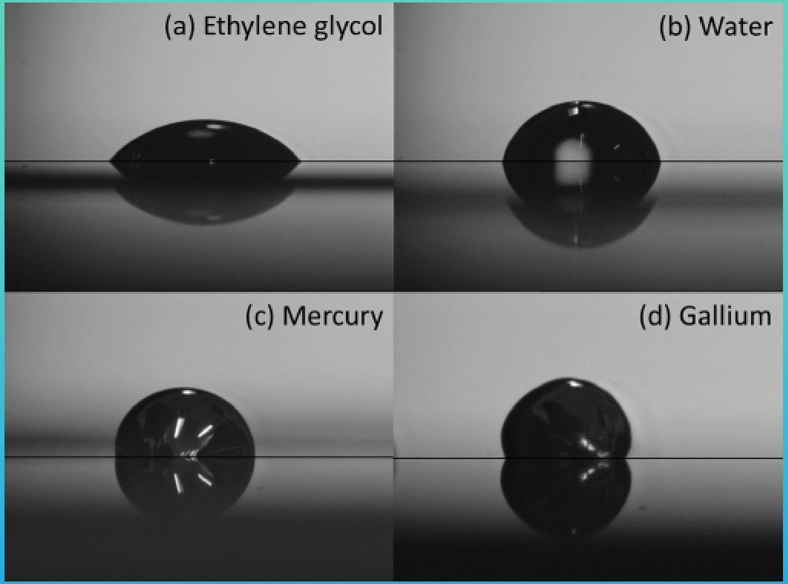
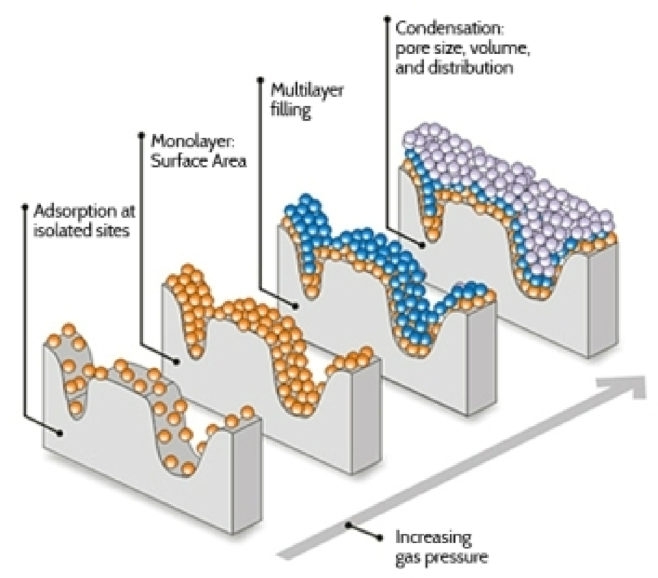
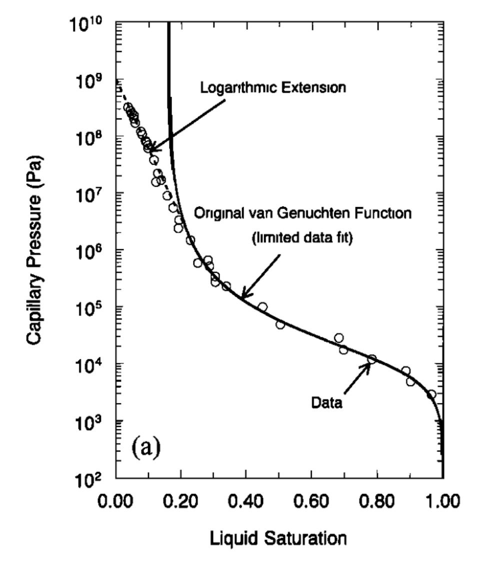
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

SAND2021-5985PE

Spent Fuel and Waste Science and Technology (SFWST)







Lightning Talk : Capillary Pressure Relationships

SFWST Annual Meeting
Tuesday May 18, 2021 (11:00-12:30)

Matthew J. Paul
Sandia National Laboratories

Capillary Pressure Non-linearities

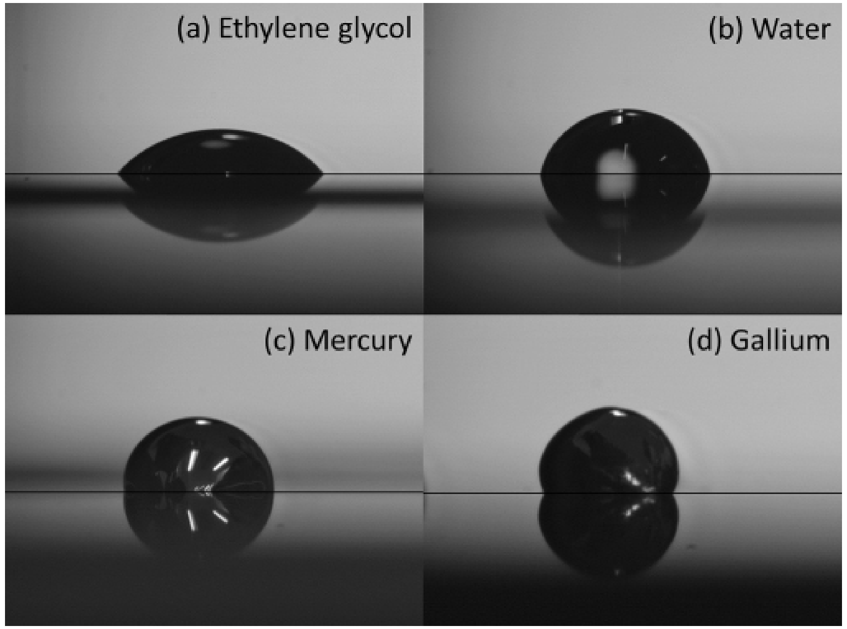
Capillary “pressure” is a form of “matrix potential”, the free energy of the fluid in a matrix relative to the bulk fluid.

$$\frac{P_c(S_w)}{\rho} = \psi_{matrix} = \psi_{adhesion} - \psi_{cohesion}$$

It can be positive or negative.

Multiple non-linear aspects of one function:

1. Hysteresis $S_w(A_{ad}, A_{co})$
2. Adhesion $\psi_{adhesion}(A_{ad})$
3. Cohesion $\psi_{cohesion}(A_{co})$



[1] Guisbiers, Arscott, and Snyders (2012). “An accurate determination of the surface energy of solid selenium” *Appl. Phys. Let. 101*

Hysteresis and Cohesion

Saturation is **convenient,** but **imperfect** state variable for matrix potential.

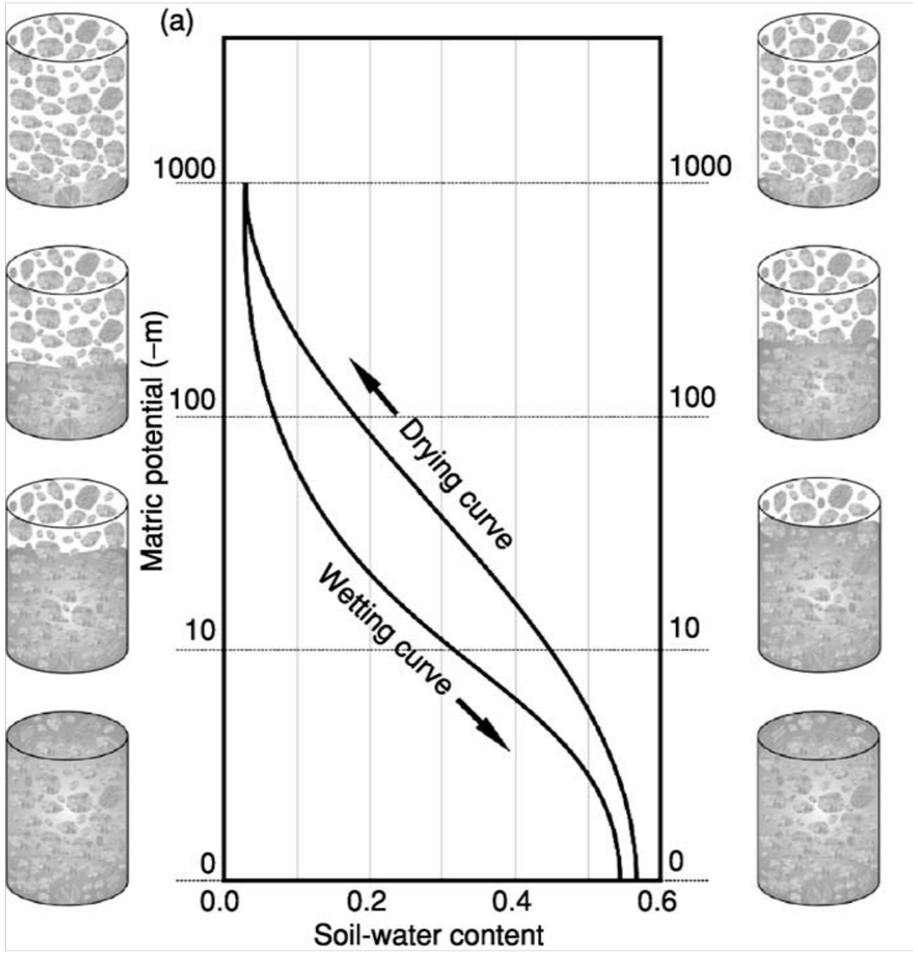
There is no **one-to-one** mapping of saturation to interfacial areas.

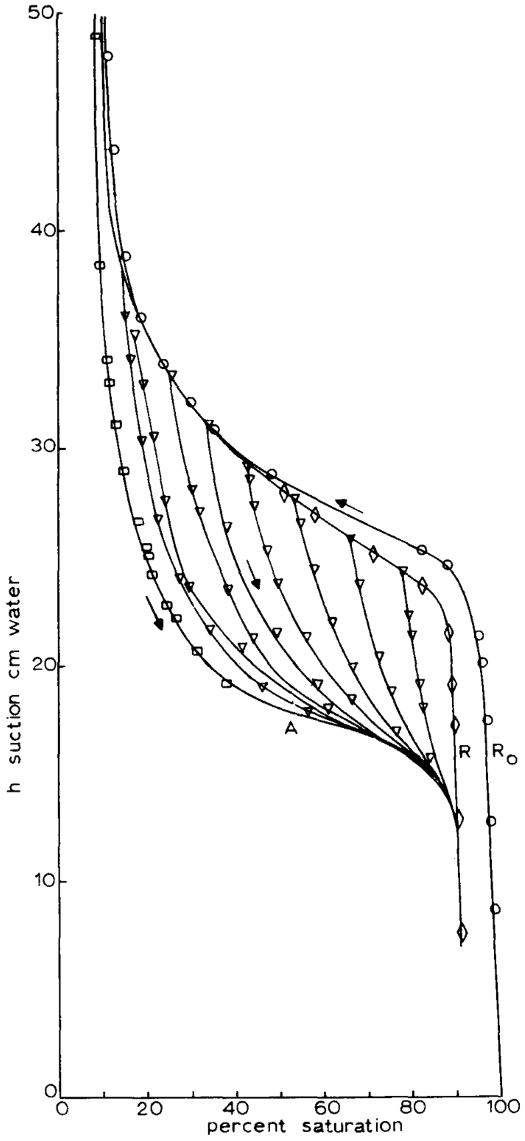
Different **interfacial areas** are created during imbibition and draining.

Small pores have large adhesion areas but very small cohesive areas

- First filled by wetting fluids (H_2O)
- Last filled by non-wetting fluids (Hg)

Matrix potential increases dramatically at the “irreducible” or “residual saturation…

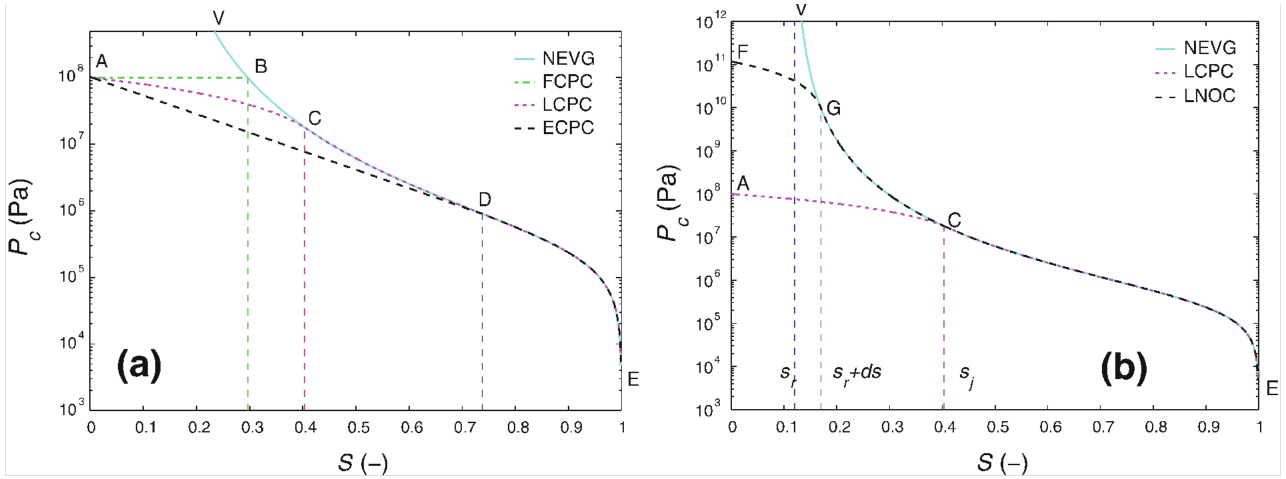




[1] Tuller and Or (2005). “Water retention and characteristic curve.” *Encyclopedia of Soils in the Environment.* Elsevier.

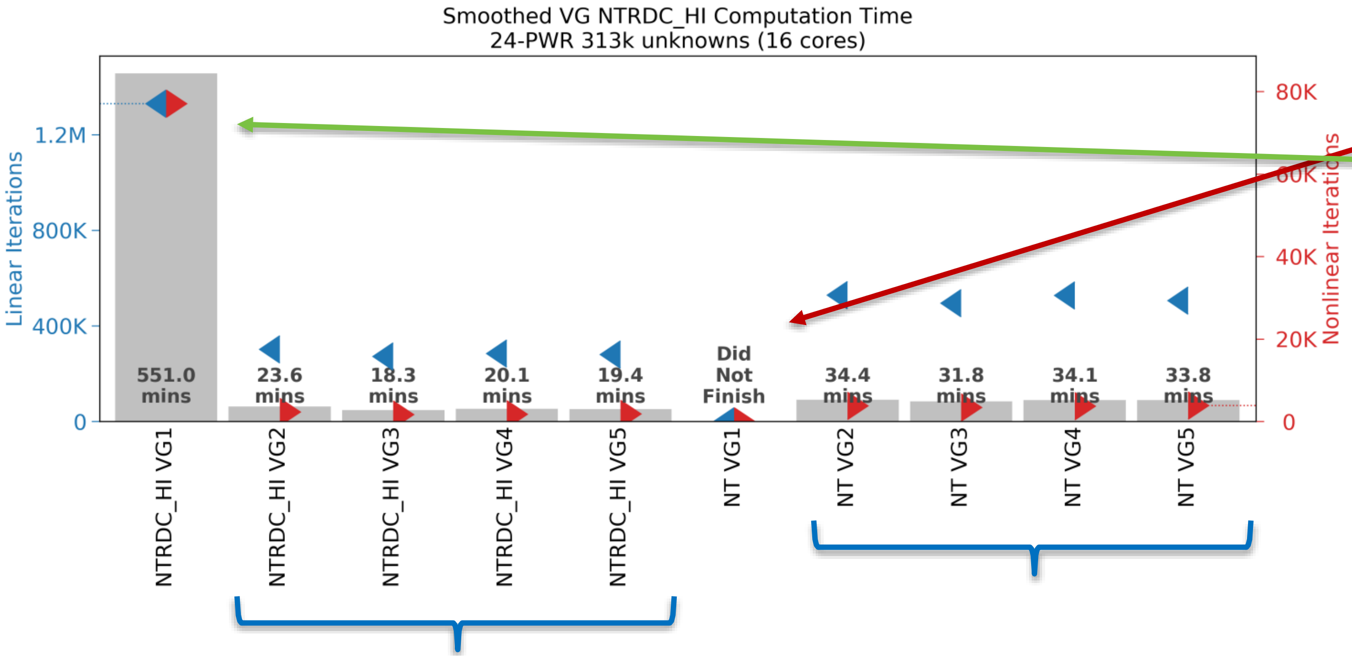
[2] Morrow and Harris (1965). “Capillary equilibrium in porous materials.” *SPE J. 5. 15-24*

Unsaturated Behavior



What happens to ”capillary pressure” at below “irreducible”? Van Genuchten is undefined.

[1] Sun et al (2010). “Modeling Thermal-Hydrologic Processes for a Heated Fractured Rock System: Impact of a Capillary-Pressure Maximum.” *Transp Porous Med* 83



Currently developing approaches to model this regime.

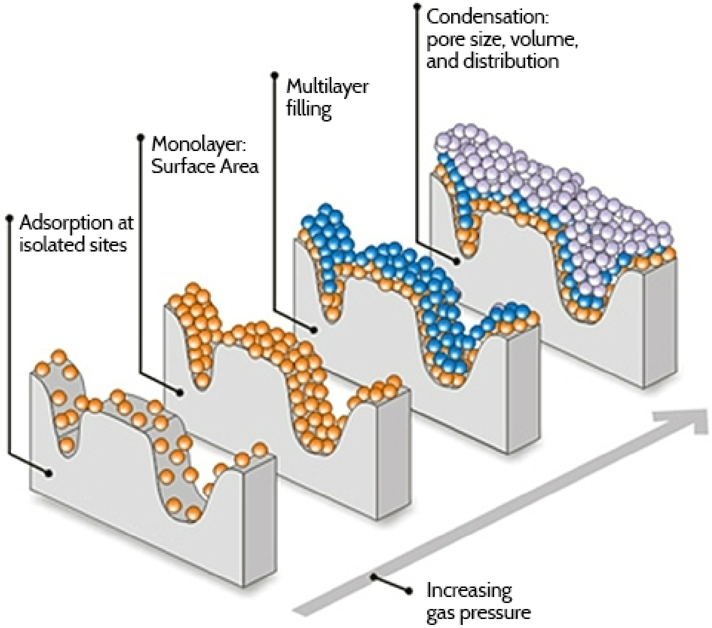
1. Solver convergence
   - Ordinary Newton (NT) solvers are unstable at cusps (VG1).
   - Newton Trust Region Dogleg-Cauchy (NTRDC) is stable.
     (Development by Heeho Park)

2. Unsaturated extensions to van Genuchten
   - “All of the above” approach to compare models
   - Smooth, piecewise extensions perform much better.

Can these extensions be physically justified?

Adsorption limits maximum “capillary pressure”

- Matrix potential energy is that in excess of liquefaction
  - $\frac{\Delta P_c}{\rho}(S_w = 0) = \Delta H_{ad}(0) - \Delta H_{liq}$
- BET theory supports interpolation
  - ΔH Monolayer > ΔH Multilayer > ΔH Bulk Condensate
  - ”Capillary pressure” diminishes with increasing saturation



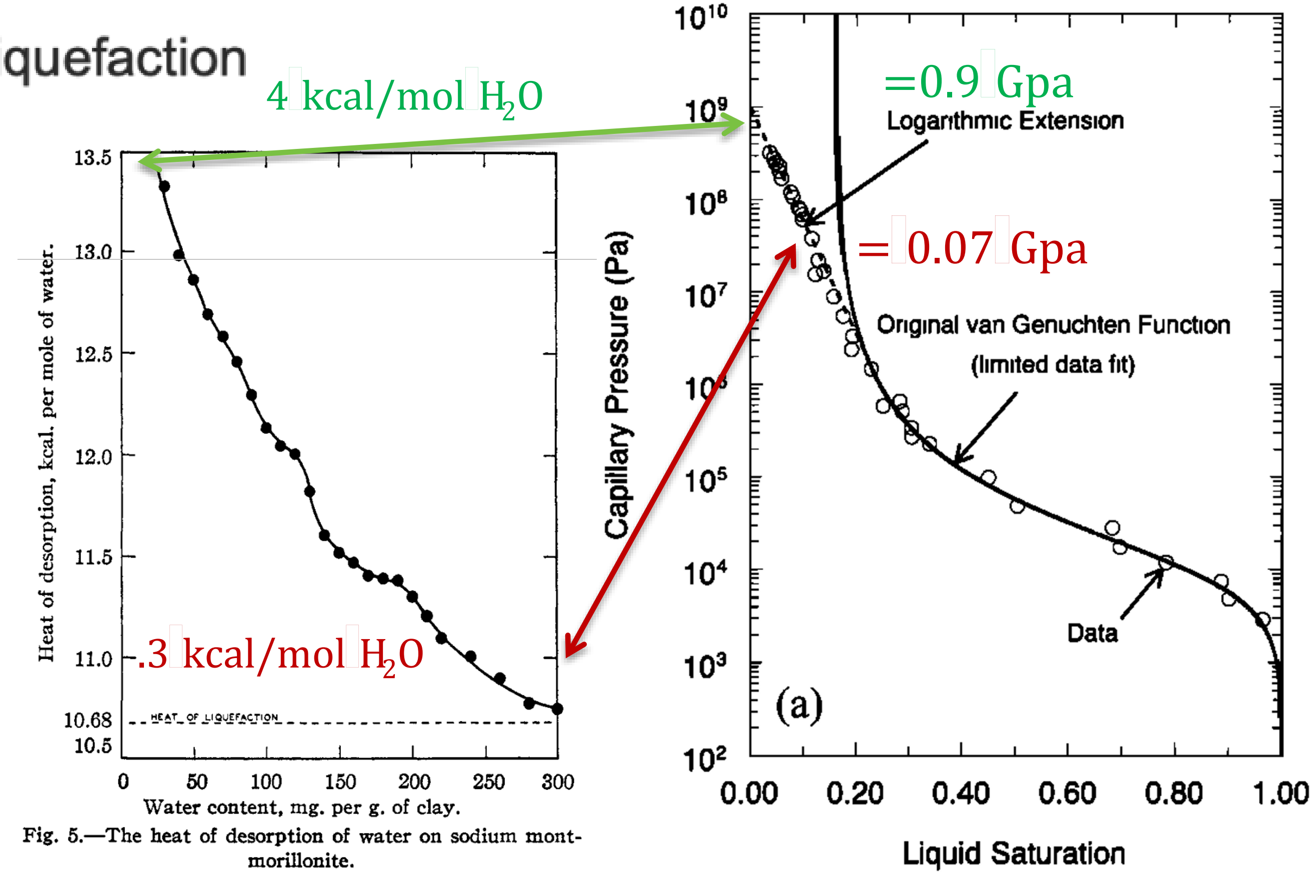


Fig. 5.—The heat of desorption of water on sodium montmorillonite.

- A maximum with interpolated slope is justified

[1] Image from micromeritcs.com

[2] Mooney, Keenan, and Wood (1952). “Adsorption of Water Vapor by Montmorillonite. I. Heat of Desorption and Application of BET Theory” *J Am Chem Soc* 74, 6.

[3] Webb (2000). “A simple extension of two-phase characteristic curves to include the dry region” *Water Resource Res* 36, 6.