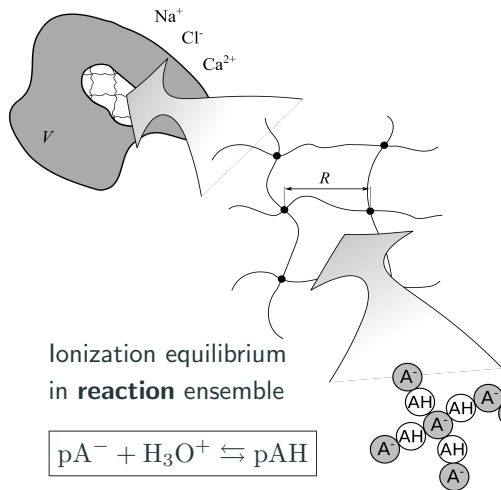


Grand-reaction ensemble.



Constant salinity

$$c_s = c_{\text{Cl}}^- = c_{\text{Na}}^+$$

The simulation box freely
exchanges ions with reservoir
as in **grand canonical**
ensemble

Landsgesell, J., Hebbeker, P., Rud, O., Lunkad, R., Koovan, P.,
Holm, C. (2020). **Grand-Reaction Method for Simulations of Ionization**

Equilibria Coupled to Ion Partitioning. Macromolecules, 53(8), 30073020.