Numerical (Aqueous) Solutions : Diffusion under Chemical Constraints

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The proton concentration in aqueous solutions is crucial in most physico-chemical reactions, and especially in physiology. Indeed, the very activity of any living cell is possible only for a limited range of pH. Nonetheless, the computation of $[H^+]$ is always challenging, not only for steady-states, but also for transient states, since most of the time, the exact kinetic schemes of all the involved chemical reactions are not known.

Recently, we successfully derived a new method to derive the computation of all protic concentrations within a cell[1]. We based our derivation on time-scales separation between the relaxation times of those reactions and the typical rates of biochemical effectors.

This later approach may be used as well for diffusion. After an investigation of the different transformation pathways for proton in aqueous solutions, we will show how to compute a fully tensorized and chemically compliant diffusion equation for all the species. We will also show that this novel algebraic method provides some results that are indistinguishable from classical methods, both on numerical tests and on experimental results. And, as a side effect, since we removed the stiffness of the underlying differential equations, we will show that we compute those results about 100 times faster than what could be achieved so far, leading to the possibility to carry out some physiological computations in very short times.

Références

1. Y. Bouret and M.Argentina and L.Counillon, Capturing intracellular pH dynamics by coupling its molecular mechanisms within a fully tractable mathematical model *PLoS One*, DOI :10.1371/journal.pone.0085449, 2014