**>> Acid-base reactions (solve\_pH() & controlpH() functions)**

A sub-model is added to this individual-based model to comprehensively describe the pH dynamics of the system. The influent enters in the reactor at a fix pH with a buffer of anions and cations. Then, in the system and due to the microbial activity, the pH varies function of the space and time (pHi,jn). As the acid-base reactions have a fast kinetics, they can be considered instantaneous, and it is possible to use and algebraic algorithm to approximate it each time step of the integration.

To describe the acid-base reactions taking place, first it is needed to define the chemical species considered and their forms. The chemical species are the states of the model: the soluble components that the user is interested to integrate. And some of these chemical species have different chemical forms in water function of the acid-base reactions associated to them. The concentration of these forms is function of the pH of the liquid as the neutrality of charges is maintained in the liquid.

Each of the forms included in the model is associated to its charge and its Gibbs energy value. This allows to directly calculate the acid-base constants for all the chemical species in the solution and to compute the balance of charges in the liquid bulk (equation 1). Because the equilibrium of charges occurs at a fast time scale, this balance is assumed to remain neutral. Therefore, it is used to calculate the pH and the concentration of all the forms of the states, finding the root of equation 24 using an implicit Newton-Raphson scheme.

(1)

Where K is the total number of all the chemical forms present in the liquid bulk, Ck is the concentration of each of the forms, and zk is its charge. To find the root of the equation 24, it is needed to write the concentrations of the forms function the concentration of protons and the states of the model (ɸi,jn), calculated through equation 1. The equations for each of the chemical forms are present in equations 2-7.

Not hydrated form concentration: (2)

Hydrated and fully protonated form concentration: (3)

First deprotonated form concentration: (4)

Second deprotonated form concentration: (5)

Third deprotonated form concentration: (6)

(7)

Where Kd, Ka1, Ka2 and Ka3 are the hydration and acid-base equilibrium constants calculated using the Gibbs energy values of formation of the substrate(s) and product(s).

**> Demonstration of equations 2-7.**

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**· (Kd) + (Ka1):**

**· (Ka2) + (Ka3):**

**· CT = *f* ([B-]):**

**· [A], [B], [B–], [B2–], [B3–] = *f* ([CT], [H+]):**

In code:

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