fermentation

H_2S Emission and Microbial Community of Chicken Manure and Vegetable Waste in Anaerobic Digestion: A Comparative Study

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File S1: Calculation process of the equilibrium from sulfide to H_2S in the liquid phase

According to the law of dissolution equilibrium, K_{s1} and K_{s2} can be defined as follows,

$$H_2S \rightleftharpoons HS^- + H^+ \implies K_{S1} = \frac{[HS^-][H^+]}{[H_2S]}$$

$$S^- \rightleftharpoons S^{2-} + H^+ \implies K_{S2} = \frac{[S^{2-}][H^+]}{[HS^-]}$$

where $[HS^-]$, $[H^+]$, and $[H_2S]$ represent the molar concentrations of HS^-, H^+, and H_2S. The soluble sulfide molar concentration was defined as $[S_T]$:

$$[S^{2-}] + [HS^-] + [H_2S] = [S_T]$$

According to the charge balance equation:

$$[H^+] = [HO^-] + [HS^-] + 2[S^{2-}]$$

$$pH = -\lg[H^+] \Rightarrow [H^+] = 10^{-pH}$$

$$pH = -\lg\frac{10^{-14}}{[HO^-]} \Rightarrow [HO^-] = \frac{10^{-14}}{10^{-pH}} \approx 0$$

(the pH value is between 5.8 and 7.3 in this study, thus, $[HO^-]$ was very low and close to zero)

$$[HS^-] + 2[S^{2-}] = 10^{-pH}$$

$$[S^{2-}] + [HS^-] + [H_2S] = [S_T]$$

$$\frac{K_{S1}}{10^{-pH}} = \frac{[HS^-]}{[H_2S]}$$

$$\frac{K_{S1}K_{S2}}{(10^{-pH})^2} = \frac{[HS^-][S^{2-}]}{[HS^-][H_2S]} = \frac{[S^{2-}]}{[H_2S]}$$

$$1 + \frac{K_{S1}}{10^{-pH}} + \frac{K_{S1}K_{S2}}{10^{-2pH}} = \frac{[H_2S] + [HS^-] + [S^{2-}]}{[H_2S]} = \frac{[S_T]}{[H_2S]}$$

$$[H_2S] = \frac{[S_T]}{1 + \frac{K_{S1}}{10^{-pH}} + \frac{K_{S1}K_{S2}}{10^{-2pH}}}$$