**Figure 1:**

(a) pH (predicted in this study) as a function of pH (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).

(b) pH (predicted in this study) as a function of pH (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).

(c) ε(NO3⁻) (predicted in this study) as a function of ε(NO3⁻) (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).

(d) ε(NH4⁺) (predicted in this study) as a function of ε(NH4⁺) (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).

(e) ε(NO3⁻) (predicted in this study) as a function of ε(NO3⁻) (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).

(f) ε(NH4⁺) (predicted in this study) as a function of ε(NH4⁺) (fixed NH simulations) for different fixed NH3 concentrations (0, 5, 10, 20, 40 ppb).