A biofilm model was developed to describe the simultaneous NO$_3^-$ and SeO$_4^{2-}$ reduction in a H$_2$-based membrane biofilm reactor (MBfR). Model calibration and validation was conducted using the experimental data of a reported H$_2$-based MBfR. With a good level of identifiability, the SeO$_4^{2-}$ affinity constant and the SeO$_3^{2-}$ affinity constant were estimated at 9.80±0.51gSem$^{-3}$ and 1.83±0.38gSem$^{-3}$, respectively. The model was then applied to evaluate the effects of key operating conditions on the single-stage H$_2$-based MBfR and the role of reactor configuration through comparing two-stage to single-stage MBfR systems. The results showed that (i) high SeO$_4^{2-}$ or low NO$_3^-$ concentration in the influent favored the growth of selenate-reducing bacteria (SeRB) and therefore benefited the Se removal, (ii) the influent dissolved oxygen slightly inhibited the Se removal through enhancing the aerobic microbial respiration on H$_2$, (iii) the H$_2$ supply should be controlled at a proper level to avoid SeRB suppression and H$_2$ wastage, (iv) thin biofilm should be avoided to ensure a protected niche for SeRB and therefore a promising Se removal, and (v) the two-stage MBfR configuration offered relatively higher efficiency in removing Se and NO$_3^-$ simultaneously under the same loading condition.