**List of parameters**

**List of equations**

𝑝𝐻 𝑒𝑥𝑡𝑒𝑛𝑠𝑖𝑜𝑛

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Keq** | **ν** | **σ** | **n** | **s** | **β** | **Ks** | **Kp** |
| **SMA** |  |  |  |  |  |  |  |  |
| **SMA Ext.** |  |  |  |  |  |  |  |  |
| **Ottens** |  |  |  |  |  |  |  |  |
| **Ottens Ext.** |  |  |  |  |  |  |  |  |
| **SMA/HIC** |  |  |  |  |  |  |  |  |
| **SMA/HIC Ext.** |  |  |  |  |  |  |  |  |

**Summary of isotherm parameters for all isotherm models. Parameters included in model framework are highlighted in green. Parameters excluded from model framework are highlighted in red.**

**References**

[1] Brooks, C. A., & Cramer, S. M. (1992). Steric mass‐action ion exchange: Displacement profiles and induced salt gradients. *AIChE Journal*, *38*(12), 1969-1978.

[2] Huuk, T. C., Hahn, T., Doninger, K., Griesbach, J., Hepbildikler, S., & Hubbuch, J. (2017). Modeling of complex antibody elution behavior under high protein load densities in ion exchange chromatography using an asymmetric activity coefficient. *Biotechnology journal*, *12*(3), 1600336.

[3] Rischawy, F., Saleh, D., Hahn, T., Oelmeier, S., Spitz, J., & Kluters, S. (2019). Good modeling practice for industrial chromatography: mechanistic modeling of ion exchange chromatography of a bispecific antibody. *Computers & Chemical Engineering*, *130*, 106532.

[4] Mollerup, J. M., Hansen, T. B., Kidal, S., & Staby, A. (2008). Quality by design—thermodynamic modelling of chromatographic separation of proteins. *Journal of Chromatography A*, *1177*(2), 200-206.

[5] Nfor, B. K., Noverraz, M., Chilamkurthi, S., Verhaert, P. D., van der Wielen, L. A., & Ottens, M. (2010). High-throughput isotherm determination and thermodynamic modeling of protein adsorption on mixed mode adsorbents. *Journal of Chromatography A*, *1217*(44), 6829-6850.

[6] Wang, G., Hahn, T., & Hubbuch, J. (2016). Water on hydrophobic surfaces: mechanistic modeling of hydrophobic interaction chromatography. *Journal of Chromatography A*, *1465*, 71-78.

[7] Lee, Y. F., Graalfs, H., & Frech, C. (2016). Thermodynamic modeling of protein retention in mixed-mode chromatography: An extended model for isocratic and dual gradient elution chromatography. *Journal of Chromatography A*, *1464*, 87-101.