**Colloidal Multi component model**

if the sum of all bound components is

 (1)

For phase ratio(COL\_PHI) [m2 /m3 (surface area/solid phase vol), Coordination number (COL\_CORDNUM =6 for hexagonal packing) for nearest neighbours,the surface coverage factor *R*,

 (2)

and screening term (nm-1) Where, , , and , are constants and *C*0 is total ionic strength

 (3)

) (4)

\*j is summed only over bound components only.

More details can be found in the paper**,** <https://doi.org/10.1016/j.chroma.2009.06.082>

Where, *r*i (m) is the radius of the protein, *K*kin (s-1)in the reaction kinetic. and are protein resin (binding equilibrium) and protein- protein interaction terms.

If the surface concentration is close to zero (COL\_LINEAR\_THRESHOLD), linear model is implemented

) (5)

To make the model dependent on ionic strength*)*  and pH, and is varied as function of pH and ionic strength

*lnK*e,i = *k*e,i (*k*a,i*-k*b,i + *k*c,i exp()(6)

*b*pp,i = *b*e,i (*b*a,i*b*b,i + *b*c,i exp()(7)

where *k*a-e, *b*a-e are fitting constants.

*lnK*e and *B*pp have no units, *K*e,i  is equilibirium constant,. bpp is protein-protein interaction term. Units for IS*)*, protein concentration in mM. pH is log of [H+] in mM. Both the Ionic strength (*)* and pH(*)*  is non- bound components.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Data set | Description | Unit | Type | Range | Length |
| COL\_PHI | Phase ratio | m2 msp-3 | double | double | 1 |
| COL\_KAPPA\_EXP | scrrening term exponent factor | - | double | double | 1 |
| COL\_KAPPA\_FACT | scrrening term factor | nm(mM)-1 | double | double | 1 |
| COL\_KAPPA\_CONST | scrrening term constant | nm | double | double | 1 |
| COL\_CORDNUM | Coordination number | - | int | >0 | 1 |
| COL\_LOGKEQ\_PH\_EXP | Equilibrium constant factor exponent term for pH | - | double | double | NTOTALBND |
| COL\_LOGKEQ\_SALT\_POWEXP | Equilibrium constant power exponent term for salt | - | double | double | NTOTALBND |
| COL\_LOGKEQ\_SALT\_POWFACT | Equilibrium constant power factor term for salt | - | double | double | NTOTALBND |
| COL\_LOGKEQ\_SALT\_EXPFACT | Equilibrium constant exponent factor term for salt | - | double | double | NTOTALBND |
| COL\_LOGKEQ\_SALT\_EXPARGMULT | Equilibrium constant exponent multiplier term for salt | - | double | double | NTOTALBND |
| COL\_BPP\_PH\_EXP | BPP constant exponent factor term for pH | - | double | double | NTOTALBND |
| COL\_BPP\_SALT\_POWEXP | Bpp constant power exponent term for salt | - | double | double | NTOTALBND |
| COL\_BPP\_SALT\_POWFACT | Bpp constant power factor term for salt | - | double | double | NTOTALBND |
| COL\_BPP\_SALT\_EXPFACT | Bpp constant exponent factor term for salt | - | double | double | NTOTALBND |
| COL\_BPP\_SALT\_EXPARGMULT | Bpp constant exponent multiplier term for salt | - | double | double | NTOTALBND |
| COL\_RADIUS | Protein radius | m | double | double | NTOTALBND |
| COL\_KKIN | Adsorbption kinetics | s-1 | double | double | NTOTALBND |
| COL\_LINEAR\_THRESHOLD | Linear threshold | - | double | double | 1 |
| COL\_USE\_PH | pH include or not | - | int | 0/1 | 1 |