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Mini Review

Thermodynamics of Irreversible Process, Computerized Animated Visualization for Multi Component Mass Transport Sorption Problems in Nanocomposites

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Mini Review

There is presented the author's mini Review of the realized theoretical investigation of the Multi (n=6)-component Mass Transfer (MMT) kinetics of the process inside the modern combined sorption "Nano-Composite" (NC) materials. The visual NC examples considered in the author's manuscripts may be represented by the selective bi-functional NC as the "Metal^0-Ion Exchangers (IEx)" planar NC L-membrane matrix where the inner active zero charged "NP^0-nano-sites" (i.e. Nano Particles, Me^0-agglomerates) are imbedded into the final combined NC-IEx sorption matrix resulting after the preliminary synthesis of the final NC L-matrix considered. The computer simulation for the modelling of the MMT NC kinetics is based here on the foundations of the irreversible thermodynamics such as multi(n)-component mass balance n (6)-Eqns. in partial differentials characterized fundamentally by the $^{new}k^{(2)}$ (6)-"thermodynamic variance" (k-parameter). The $k^{(2)}$-"variance parameter" describes the well kown thermodynamic "degree of freedom" of the multi(n=6)-component MMT NC kinetic system considered. The another fundamental characteristics of the irreversible thermodynamics are also included, namely the key wave concept (W) of the propagating mode of the multi (n=6)-component $\{X_n(L,T)\}$-concentration waves-distributions (n=1,2,..6); Mass Action Laws (MAL_S); "sink-source" mass transformation selective mechanism during the MMT NC kinetic process; the fundamental Nernst-Plank flux equations, electro-neutrality relations and some others.

The theoretical computer simulation is based on the two various bi-functional $k^{(1,2)}$-NC Models elaborated for MMT NC kinetics previously ($^{prev}k^{(1)}=5$), and in this manuscript ($^{new}k^{(2)}=6$). The computer simulation based on the expanded $^{new}k^{(2)}(6)$-NC Model here brings the final results: the propagating mode of the multi (n=6)-component $\{X_n(L,T)\}$-concentration waves-distributions in the NC L-membrane. The multi-component (n=6) $\{X_n(L,T)$-concentration waves describe the MMT NC kinetics on the basis of the fundamental wave (W)-concept mentioned.

The n(6)-components of the $\{X_n\}$-concentration composition ($n=_{1,2}(R^0p)^+; {}_{(3,4)}p^+; j^-_5; {}_6R^0$) are participants of the MMT NC kinetics inside the bi-functional NC planar L-matrix with the two co-existing ($I_{1,2}$&II-MMT routes), and put together the MMT $^{new}k^{(2)}(6)$-NC Model elaborated. The expanded MMT NC system considered with the new bi-functional $^{new}k^{(2)}(6)$-NC Model comprises the four $\{_{3,4}p^X{}_{m1,2}(R^0p)\}=\{2_p{}^X2_m\}$-principal paired components-participants, namely the two diffusing $_{(3,4)}p^+$-sorbate ions-principals ($D_{3,4}>0$) together with the corresponding fixed $m_{1,2}$-principals ($D_{1,2}=0$) participated in the sorption(Ia⇀)-desorption(Id↽)stages of the ($I_{1,2}$)-selective MAL_S reactions. The details of the MMT bi-functional ($I_{1,2}$-Selectivity & Diffusivity, II) $^{new}k^{(2)}$-NC Model are illustrated via the conceptual visual diagrams in the full author's publications [SM&EI J. v.2,N4, 2018 pp.128-132; MAMS J. 2019, in preparation]. The availability of the five $\{m_{1,2}; {}_{(3,4)}p; {}_6R^0\}$-principal components namely, the four paired $\{2_p{}^X2_m\}$-principals including the last introduced and crucial ($_{k=6}R^0$)-principal 6th-component which is fundamentally important for the investigation of the interference of the peculiar $\{X_{1,2,6}(L,T)\}$-travelling concentration waves calculated during the computer simulation elaborated. The key fundamental principal component ($_6R^0$) denotes the $_6R^0$- "NP^0-nanosites" with

the various $[_6R^0]$-concentrations of the "NP^0-nanosites" (see above). The cardinal, fixed $_6R^0$-principal in the NC L-membrane is introduced purposely into the theoretical MMT NC kinetic system consideration in the full version of the author's manuscript [MAMS J., in preparation]. In addition to the $(I_{1,2})$-MMT selective route in the NC matrix it is included into consideration the second, $\{D_{3-5}\}$-multi-Diffusion (II)-MMT co-route for the two diffusing $_{(3,4)}p^+$-sorbate principals with taking into account the diffusing $(D_5>0)$ 5^{th}-co-ions (j^-_5). The j^-_5-co-ionic component maintains the electro-neutrality in the bi-functional combined MMT NC system namely, $(I_{1,2})$-selective sorption (for sorbed $m_{1,2}$)&(II)-$\{D_{3-5}\}$-multi-Diffusion (for $_{(3,4)}p^+,j^-_5$-components, $D_{3-5}>0$) described in the full version of the author's manuscripts [MS&EI ; MAMS J.,in preparation]. The interference of the peculiar $\{X_{1,2,6}(L,T)\}$-travelling concentration waves during the computer simulation brings the chromatographic Displacement Development (DD)-behavior of the two interfering $X_1(L,T)$-displacer, and $X_2(L,T)$-displaced concentration waves [MS&EI J. 2].For the MMT NC kinetics there is displayed visually (via the multi-colored "captured video", illustrated in the full versions [MS&EI J. v.2(4) 2018; MAMS J., in preparation, 2019] that the reason for the atypical and peculiar $\{X_{1,2,6}(L,T)\}$-concentration waves behavior consists in the combined property expressed by the bi-functionality of the NC matrix via the combination of the (selectivity, $I_{1,2}$) & (II, Diffusivity)-MMT co-routes considered. The influence of the two principal $_{(3,4)}p^+$-sorbate participants-diffusants properties (with $D_{3,4}>0$-mobility) is transferred to the peculiar $X_{m(1,2)}$ (L,T)-concentration waves for the in-diffusible $_{m(1,2)}(Rp)^+$-principal components-complexes (where $D_{1,2}=0$). The several illustrations and References for the given mini-Review including the structure of the NC bi-functional matrices; the various (peculiar$_{1,2,6}$ and diffusing$_{3,4}$) multi(n)-components $\{X_n(L,T)\}$-principal concentration waves, and finally "pictures-frames" of the travelling $\{X_n(L,T)\}$-concentration waves are presented in the author's manuscripts mentioned above.

Conclusion

a) Computer simulation by the mass balance n(6)-Eqns. for a number of variants includes the contemporary and bi-functional Nano-Composite, $k^{(2)}(6)$-NC Models elaborated.

b) Numerical results of the computerized modeling bring the interference of the multi-n(6)-component $\{X_n(L,T)\}$- travelling concentration waves in the NC planar L-membrane.

c) Phenomenological wave W-concept is extended to a sorption M(n=6)MT phenomena in the bi-functional L-NanoComposites (NC).

d) Visual computerized sci. animations created show clearly the interference of the Xn-concentration waves for the paired 3,4p & m1,2-principal components sorbed onto 6R0-nano-sites.

e) Computerized Visualized Simulation results show the interference of the principal peculiar {X1,2,6(L,T)}-waves in the NC via the phenomenological wave (W)-concept.

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